



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:19 PM UTC

PDB ID : 4U4R / pdb\_00004u4r  
Title : Crystal structure of Lactimidomycin bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

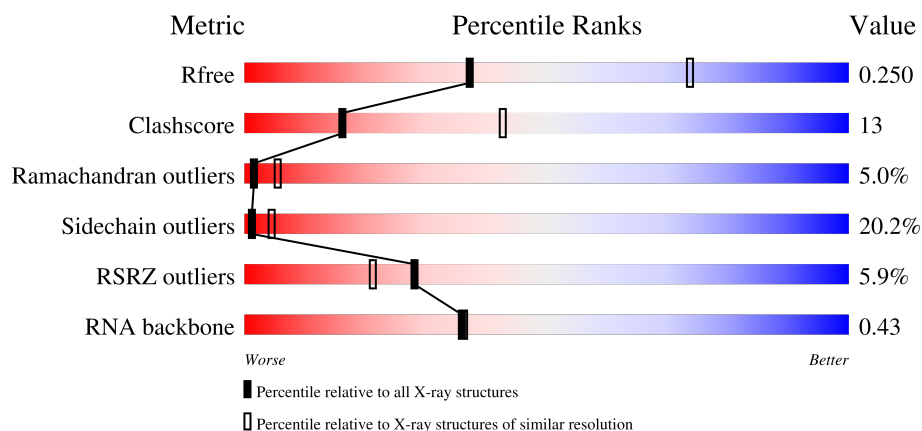
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



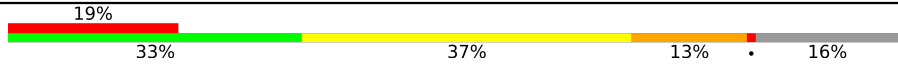
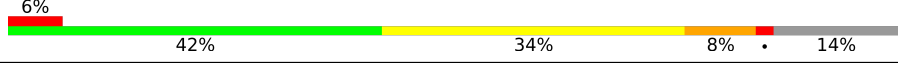
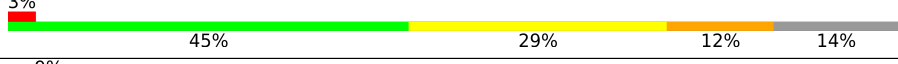
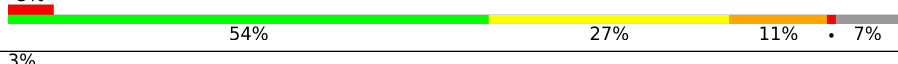
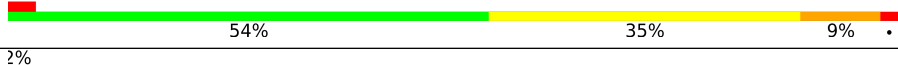
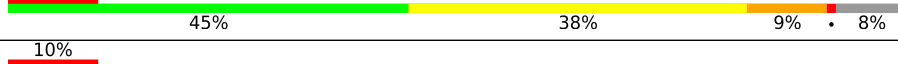
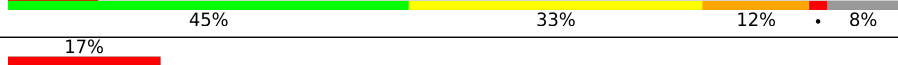
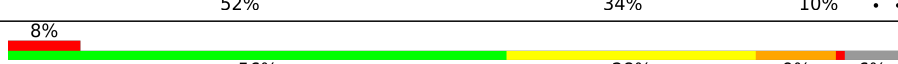
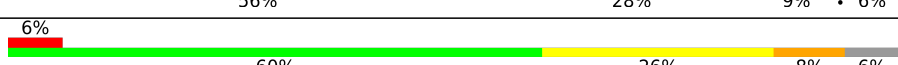
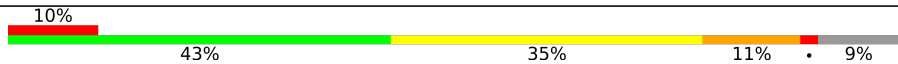
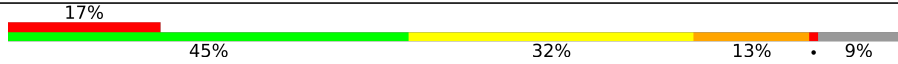
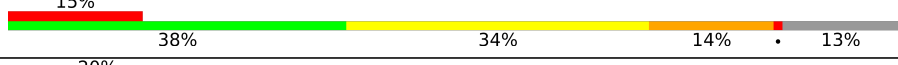
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |
| RNA backbone          | 3983                        | 1114 (3.00-2.60)                                      |

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

| Mol | Chain | Length | Quality of chain                                         |
|-----|-------|--------|----------------------------------------------------------|
| 1   | 2     | 1800   | <div> <div>5%</div> <div>45% 38% 14% .</div> </div>      |
| 1   | 6     | 1800   | <div> <div>5%</div> <div>48% 38% 14%</div> </div>        |
| 2   | S0    | 251    | <div> <div>15%</div> <div>29% 39% 13% . 18%</div> </div> |
| 2   | s0    | 251    | <div> <div>8%</div> <div>39% 32% 10% . 18%</div> </div>  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | S1    | 254    |    |
| 3   | s1    | 254    |    |
| 4   | S2    | 253    |    |
| 4   | s2    | 253    |    |
| 5   | S3    | 239    |    |
| 5   | s3    | 239    |    |
| 6   | S4    | 260    |    |
| 6   | s4    | 260    |    |
| 7   | S5    | 224    |    |
| 7   | s5    | 224    |    |
| 8   | S6    | 236    |    |
| 8   | s6    | 236    |   |
| 9   | S7    | 189    |  |
| 9   | s7    | 189    |  |
| 10  | S8    | 200    |  |
| 10  | s8    | 200    |  |
| 11  | S9    | 196    |  |
| 11  | s9    | 196    |  |
| 12  | C0    | 105    |  |
| 12  | c0    | 105    |  |
| 13  | C1    | 155    |  |
| 13  | c1    | 155    |  |
| 14  | C2    | 142    |  |
| 14  | c2    | 142    |  |
| 15  | C3    | 150    |  |

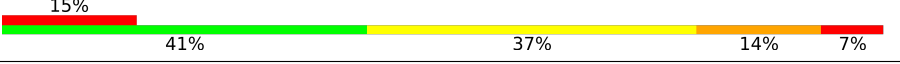
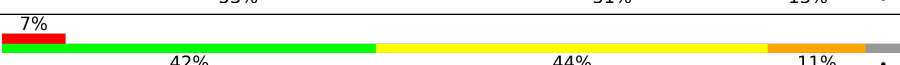
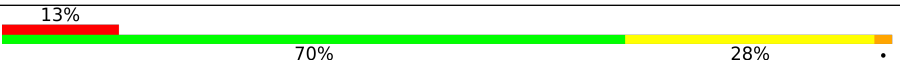
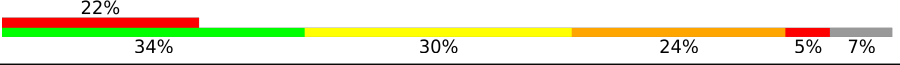
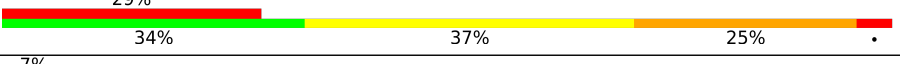
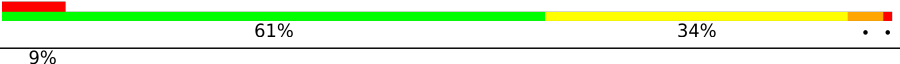
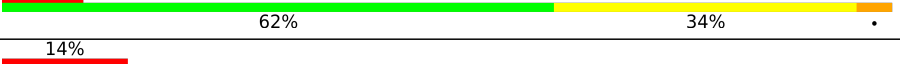
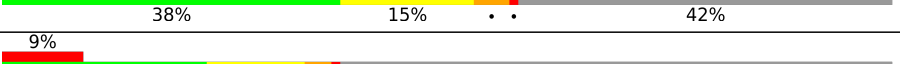
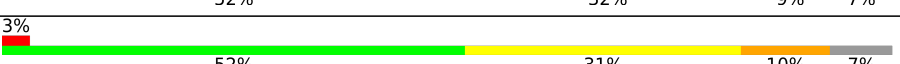
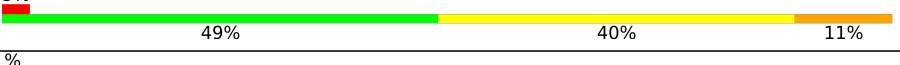
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | c3    | 150    |                  |
| 16  | C4    | 136    |                  |
| 16  | c4    | 136    |                  |
| 17  | C5    | 141    |                  |
| 17  | c5    | 141    |                  |
| 18  | C6    | 142    |                  |
| 18  | c6    | 142    |                  |
| 19  | C7    | 136    |                  |
| 19  | c7    | 136    |                  |
| 20  | C8    | 145    |                  |
| 20  | c8    | 145    |                  |
| 21  | C9    | 143    |                  |
| 21  | c9    | 143    |                  |
| 22  | D0    | 120    |                  |
| 22  | d0    | 120    |                  |
| 23  | D1    | 87     |                  |
| 23  | d1    | 87     |                  |
| 24  | D2    | 129    |                  |
| 24  | d2    | 129    |                  |
| 25  | D3    | 144    |                  |
| 25  | d3    | 144    |                  |
| 26  | D4    | 134    |                  |
| 26  | d4    | 134    |                  |
| 27  | D5    | 107    |                  |
| 27  | d5    | 107    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | D6    | 97     |    |
| 28  | d6    | 97     |    |
| 29  | D7    | 81     |    |
| 29  | d7    | 81     |    |
| 30  | D8    | 66     |    |
| 30  | d8    | 66     |    |
| 31  | D9    | 55     |    |
| 31  | d9    | 55     |    |
| 32  | E0    | 60     |    |
| 33  | E1    | 76     |    |
| 33  | e1    | 76     |   |
| 34  | SR    | 318    |  |
| 34  | sR    | 318    |  |
| 35  | SM    | 273    |  |
| 35  | sM    | 273    |  |
| 36  | 1     | 3396   |  |
| 36  | 5     | 3396   |  |
| 37  | 3     | 121    |  |
| 37  | 7     | 121    |  |
| 38  | 4     | 158    |  |
| 38  | 8     | 158    |  |
| 39  | L2    | 253    |  |
| 39  | l2    | 253    |  |
| 40  | L3    | 386    |  |
| 40  | l3    | 386    |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41  | L4    | 361    |                  |
| 41  | l4    | 361    |                  |
| 42  | L5    | 296    |                  |
| 42  | l5    | 296    |                  |
| 43  | L6    | 175    |                  |
| 43  | l6    | 175    |                  |
| 44  | L7    | 243    |                  |
| 44  | l7    | 243    |                  |
| 45  | L8    | 255    |                  |
| 45  | l8    | 255    |                  |
| 46  | L9    | 191    |                  |
| 46  | l9    | 191    |                  |
| 47  | M0    | 220    |                  |
| 47  | m0    | 220    |                  |
| 48  | M1    | 173    |                  |
| 48  | m1    | 173    |                  |
| 49  | M3    | 198    |                  |
| 49  | m3    | 198    |                  |
| 50  | M4    | 137    |                  |
| 50  | m4    | 137    |                  |
| 51  | M5    | 203    |                  |
| 51  | m5    | 203    |                  |
| 52  | M6    | 198    |                  |
| 52  | m6    | 198    |                  |
| 53  | M7    | 183    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | m7    | 183    |                  |
| 54  | M8    | 185    |                  |
| 54  | m8    | 185    |                  |
| 55  | M9    | 188    |                  |
| 55  | m9    | 188    |                  |
| 56  | N0    | 172    |                  |
| 56  | n0    | 172    |                  |
| 57  | N1    | 159    |                  |
| 57  | n1    | 159    |                  |
| 58  | N2    | 120    |                  |
| 58  | n2    | 120    |                  |
| 59  | N3    | 136    |                  |
| 59  | n3    | 136    |                  |
| 60  | N4    | 155    |                  |
| 60  | n4    | 155    |                  |
| 61  | N5    | 141    |                  |
| 61  | n5    | 141    |                  |
| 62  | N6    | 126    |                  |
| 62  | n6    | 126    |                  |
| 63  | N7    | 135    |                  |
| 63  | n7    | 135    |                  |
| 64  | N8    | 148    |                  |
| 64  | n8    | 148    |                  |
| 65  | N9    | 58     |                  |
| 65  | n9    | 58     |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 66  | O0    | 104    |                  |
| 66  | o0    | 104    |                  |
| 67  | O1    | 112    |                  |
| 67  | o1    | 112    |                  |
| 68  | O2    | 129    |                  |
| 68  | o2    | 129    |                  |
| 69  | O3    | 106    |                  |
| 69  | o3    | 106    |                  |
| 70  | O4    | 119    |                  |
| 70  | o4    | 119    |                  |
| 71  | O5    | 119    |                  |
| 71  | o5    | 119    |                  |
| 72  | O6    | 99     |                  |
| 72  | o6    | 99     |                  |
| 73  | O7    | 87     |                  |
| 73  | o7    | 87     |                  |
| 74  | O8    | 77     |                  |
| 74  | o8    | 77     |                  |
| 75  | O9    | 50     |                  |
| 75  | o9    | 50     |                  |
| 76  | Q0    | 52     |                  |
| 76  | q0    | 52     |                  |
| 77  | Q1    | 25     |                  |
| 77  | q1    | 25     |                  |
| 78  | Q2    | 105    |                  |

Continued on next page...



Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 78  | q2    | 105    |                  |
| 79  | Q3    | 91     |                  |
| 79  | q3    | 91     |                  |
| 80  | e0    | 62     |                  |
| 81  | m2    | 160    |                  |
| 82  | p0    | 311    |                  |
| 83  | p1    | 47     |                  |
| 84  | p2    | 46     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85  | MG   | 1     | 3405 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3652 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3677 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3809 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3820 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3865 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1915 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1928 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1951 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1954 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1960 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1968 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1975 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1991 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2018 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2020 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3466 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3661 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3707 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3881 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3886 | -         | -        | -       | X                |
| 85  | MG   | 6     | 1924 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2035 | -         | -        | -       | X                |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85  | MG   | 6     | 2039 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2040 | -         | -        | -       | X                |
| 85  | MG   | M3    | 203  | -         | -        | -       | X                |
| 86  | OHX  | 1     | 3943 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 3962 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 3964 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 3976 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 3980 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4007 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4023 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4032 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4036 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4047 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4048 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4056 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4059 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4060 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4061 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4065 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4071 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4084 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4088 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4089 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4118 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4143 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4149 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4153 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4157 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4158 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4159 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4163 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4166 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4175 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4177 | -         | -        | X       | -                |
| 86  | OHX  | 1     | 4200 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2032 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2045 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2076 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2084 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2086 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2090 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2091 | -         | -        | X       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86  | OHX  | 2     | 2096 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2099 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2109 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2116 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2132 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2147 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2155 | -         | -        | X       | -                |
| 86  | OHX  | 2     | 2163 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 3962 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 3973 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 3978 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4000 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4001 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4011 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4020 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4033 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4034 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4055 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4065 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4066 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4074 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4076 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4081 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4090 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4093 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4094 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4141 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4187 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4189 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4190 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4196 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4197 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4198 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4201 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4212 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4215 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4222 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4234 | -         | -        | X       | -                |
| 86  | OHX  | 5     | 4241 | -         | -        | X       | -                |
| 86  | OHX  | 6     | 2060 | -         | -        | X       | -                |
| 86  | OHX  | 6     | 2121 | -         | -        | X       | -                |
| 86  | OHX  | 6     | 2147 | -         | -        | X       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86  | OHX  | 6     | 2150 | -         | -        | X       | -                |
| 86  | OHX  | 6     | 2171 | -         | -        | X       | -                |
| 86  | OHX  | 7     | 218  | -         | -        | X       | -                |
| 86  | OHX  | 7     | 219  | -         | -        | X       | -                |
| 86  | OHX  | 7     | 224  | -         | -        | X       | -                |
| 86  | OHX  | 7     | 226  | -         | -        | X       | -                |
| 86  | OHX  | 8     | 215  | -         | -        | X       | -                |
| 86  | OHX  | 8     | 223  | -         | -        | X       | -                |
| 86  | OHX  | 8     | 224  | -         | -        | X       | -                |
| 86  | OHX  | C1    | 201  | -         | -        | X       | -                |
| 86  | OHX  | O7    | 103  | -         | -        | X       | -                |
| 86  | OHX  | O9    | 101  | -         | -        | X       | -                |
| 86  | OHX  | c1    | 202  | -         | -        | X       | -                |
| 86  | OHX  | o4    | 203  | -         | -        | X       | -                |
| 87  | ZN   | Q2    | 501  | -         | -        | X       | -                |

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411226 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 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 2     | 1750     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 37283 | 16668 | 6591 | 12274 | 1750 |         |         |       |
| 1   | 6     | 1795     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 38238 | 17095 | 6758 | 12590 | 1795 |         |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | S0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1577  | 1014 | 278 | 283 | 2 |         |         |       |
| 2   | s0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1583  | 1017 | 281 | 283 | 2 |         |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | S1    | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1709  | 1084 | 310 | 311 | 4 |         |         |       |
| 3   | s1    | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1091 | 312 | 315 | 4 |         |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | S2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |
| 4   | s2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | S3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |
| 5   | s3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | S4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |
| 6   | s4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | S5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |
| 7   | s5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | S6    | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1799  | 1129 | 346 | 321 | 3 |         |         |       |
| 8   | s6    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1102 | 337 | 313 | 3 |         |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | S7    | 184      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |  |         |         |       |
| 9   | s7    | 186      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1491  | 957 | 267 | 267 |  |         |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | s8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | S9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |
| 11  | s9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | C0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 773   | 500 | 126 | 145 | 2 |         |         |       |
| 12  | c0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 491 | 125 | 144 | 2 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |
| c0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | C1    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1214  | 775 | 230 | 206 | 3 |         |         |       |
| 13  | c1    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |
| c1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |

- Molecule 14 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | C2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 560 | 156 | 172 | 2 |         |         |       |
| 14  | c2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 560 | 156 | 172 | 2 |         |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | C3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |
| 15  | c3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | C4    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 545 | 182 | 163 | 1 |         |         |       |
| 16  | c4    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 949   | 582 | 188 | 176 | 3 |         |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | C5    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 622 | 182 | 166 | 7 |         |         |       |
| 17  | c5    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 658 | 196 | 178 | 7 |         |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18  | C6    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |         |         |       |
| 18  | c6    | 142      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1111  | 711 | 204 | 196 |         |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | C7    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 577 | 177 | 170 | 2 |         |         |       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | c7    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 906   | 563 | 174 | 167 | 2 |         |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | C8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |
| 20  | c8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | C9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |
| 21  | c9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | D0    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 855   | 539 | 156 | 159 | 1 |         |         |       |
| 22  | d0    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 882   | 554 | 161 | 166 | 1 |         |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | D1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |
| 23  | d1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | D2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |
| 24  | d2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | D3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |
| 25  | d3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | D4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |
| 26  | d4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 27  | D5    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 563   | 360 | 104 | 99 |         |         |       |
| 27  | d5    | 69       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 558   | 357 | 103 | 98 |         |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | D6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |
| 28  | d6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | D7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |
| 29  | d7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | D8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |
| 30  | d8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |
| 31  | d9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32  | E0    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 475   | 299 | 98 | 77 | 1 |         |         |       |

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | E1    | 71       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 566   | 362 | 106 | 94 | 4 |         |         |       |
| 33  | e1    | 76       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 117 | 99 | 4 |         |         |       |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34  | SR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2441  | 1544 | 419 | 470 | 8 |         |         |       |
| 34  | sR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2442  | 1544 | 418 | 472 | 8 |         |         |       |

- Molecule 35 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 35  | SM    | 159      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1104  | 652 | 221 | 231 |  |         |         |       |
| 35  | sM    | 104      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 680   | 403 | 140 | 137 |  |         |         |       |

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 36  | 1     | 3149     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67355 | 30086 | 12142 | 21978 | 3149 |         |         |       |
| 36  | 5     | 3150     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67376 | 30095 | 12145 | 21987 | 3149 |         |         |       |

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37  | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |
| 37  | 7     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 38  | 4     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |
| 38  | 8     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39  | L2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1914  | 1191 | 388 | 334 | 1 |         |         |       |
| 39  | l2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1912  | 1190 | 388 | 333 | 1 |         |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | L3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |
| 40  | l3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 41  | L4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |
| 41  | l4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42  | L5    | 296      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2375  | 1501 | 414 | 458 | 2 |         |         |       |
| 42  | l5    | 294      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2359  | 1489 | 412 | 456 | 2 |         |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | L6    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 800 | 222 | 216 | 1 |         |         |       |
| 43  | l6    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1248  | 806 | 224 | 217 | 1 |         |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 44  | L7    | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |         |       |
| 44  | l7    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1155 | 325 | 310 | 1 |         |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | L8    | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |         |       |
| 45  | l8    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1763  | 1130 | 316 | 314 | 3 |         |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | L9    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | 19    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47  | M0    | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1083 | 322 | 294 | 6 |         |         |       |
| 47  | m0    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1094 | 325 | 297 | 6 |         |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | M1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |
| 48  | m1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49  | M3    | 193      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |  |         |         |       |
| 49  | m3    | 194      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1548  | 965 | 316 | 267 |  |         |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | M4    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |         |       |
| 50  | m4    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1059  | 678 | 200 | 179 | 2 |         |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51  | M5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |
| 51  | m5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | M6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |
| 52  | m6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 53  | M7    | 183      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1420  | 882 | 281 | 257 |  |         |         |       |
| 53  | m7    | 155      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1227  | 764 | 238 | 225 |  |         |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | M8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |
| 54  | m8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 55  | M9    | 188      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |  |         |         |       |
| 55  | m9    | 188      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |  |         |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | N0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |
| 56  | n0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | N1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |
| 57  | n1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | N2    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 796   | 516 | 131 | 149 |   |         |         |       |
| 58  | n2    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 778   | 505 | 127 | 146 |   |         |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59  | N3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |
| 59  | n3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60  | N4    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 699   | 443 | 137 | 118 | 1 |         |         |       |
| 60  | n4    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1038  | 651 | 206 | 180 | 1 |         |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | N5    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 620 | 169 | 173 | 2 |         |         |       |
| 61  | n5    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 617 | 168 | 172 | 2 |         |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 62  | N6    | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |   |         |         |       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 62  | n6    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 63  | N7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |
| 63  | n7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64  | N8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |
| 64  | n8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 65  | N9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |
| 65  | n9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66  | O0    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 743   | 479 | 124 | 139 | 1 |         |         |       |
| 66  | o0    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 492 | 128 | 146 | 1 |         |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67  | O1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |         |       |
| 67  | o1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 559 | 167 | 156 | 1 |         |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | O2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |
| 68  | o2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | O3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |
| 69  | o3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70  | O4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |
| 70  | o4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71  | O5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |         |       |
| 71  | o5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 612 | 185 | 167 | 1 |         |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72  | O6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |         |       |
| 72  | o6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 481 | 156 | 131 | 2 |         |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73  | O7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |
| 73  | o7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 74  | O8    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |   |         |         |       |
| 74  | o8    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 114 | 106 |   |         |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75  | O9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |
| 75  | o9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 76  | Q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |
| 76  | q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | Q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |
| 77  | q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78  | Q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78  | q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 79  | Q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |
| 79  | q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 80  | e0    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 309 | 101 | 80 | 1 |         |         |       |

- Molecule 81 is a protein called Unknown protein m2.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 81  | m2    | 150      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 750   | 450 | 150 | 150 |  |         |         |       |

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 82  | p0    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1077  | 687 | 192 | 195 | 3 |         |         |       |

- Molecule 83 is a protein called Unknown protein p1.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 83  | p1    | 47       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 235   | 141 | 47 | 47 |  |         |         |       |

- Molecule 84 is a protein called Unknown protein p2.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 84  | p2    | 46       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 230   | 138 | 46 | 46 |  |         |         |       |

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85  | 2     | 126      | Total<br>126 | Mg<br>126 | 0       | 0       |
| 85  | S8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | C3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | SM    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | 1     | 475      | Total<br>475 | Mg<br>475 | 0       | 0       |
| 85  | 3     | 14       | Total<br>14  | Mg<br>14  | 0       | 0       |
| 85  | 4     | 21       | Total<br>21  | Mg<br>21  | 0       | 0       |
| 85  | L2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | L3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | L4    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | L5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | L6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | L7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | L8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | M0    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | M1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | M3    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 85  | M5    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | M6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | M7    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 85  | M9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85  | N0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | N3    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | N5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | N8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | O3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | Q2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | 6     | 147      | Total<br>147 | Mg<br>147 | 0       | 0       |
| 85  | s1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | s6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | s8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | c1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | c7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | c8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | d2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | d3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | d6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | sM    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | 5     | 504      | Total<br>504 | Mg<br>504 | 0       | 0       |
| 85  | 7     | 15       | Total<br>15  | Mg<br>15  | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

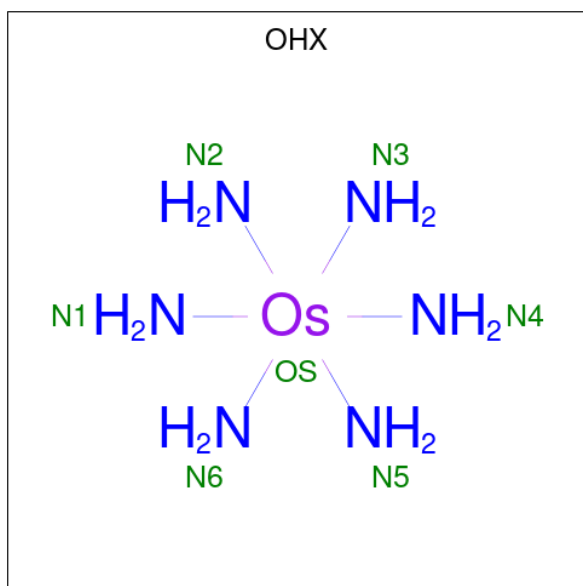
| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 85  | 8     | 13       | Total<br>13 | Mg<br>13 | 0       | 0       |
| 85  | l2    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | l3    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | l4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | l5    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 85  | l7    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | m1    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | m4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | m5    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | m6    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | m7    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 85  | n0    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | n3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | n6    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | n8    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 85  | n9    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | o1    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | o3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | o4    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 85  | q0    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 85  | q1    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 85  | q3    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 86  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | S8    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | C1    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | C3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | C5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | C8    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | D9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | SR    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L4    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L6    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M6    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | N9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | O2    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | O3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | O7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | O7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | O9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | Q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 6     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | s1    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | s1    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | s4    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | s8    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | s9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | c1    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | c3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | c5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | c8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | d4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | d9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | sR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 19    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | m6    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | n3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | n9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

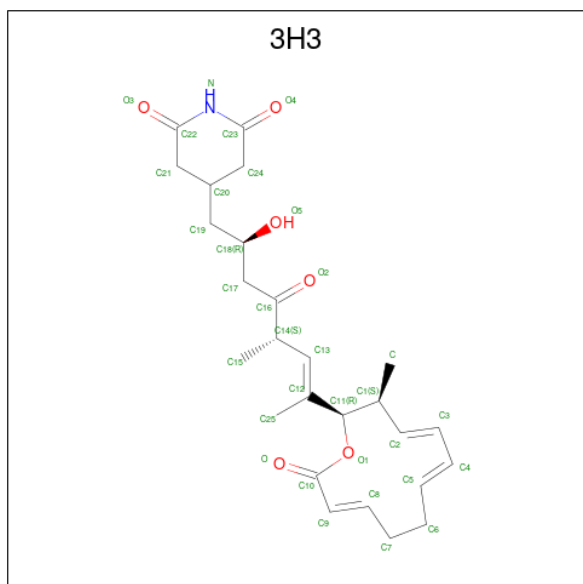
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 87  | D6    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | D7    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | D9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | E1    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | O7    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | Q0    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | Q2    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | Q3    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | d6    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 87  | d7    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | d9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | e1    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | o7    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | q0    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | q2    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 87  | q3    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (CCD ID: 3H3) (formula: C<sub>26</sub>H<sub>35</sub>NO<sub>6</sub>).

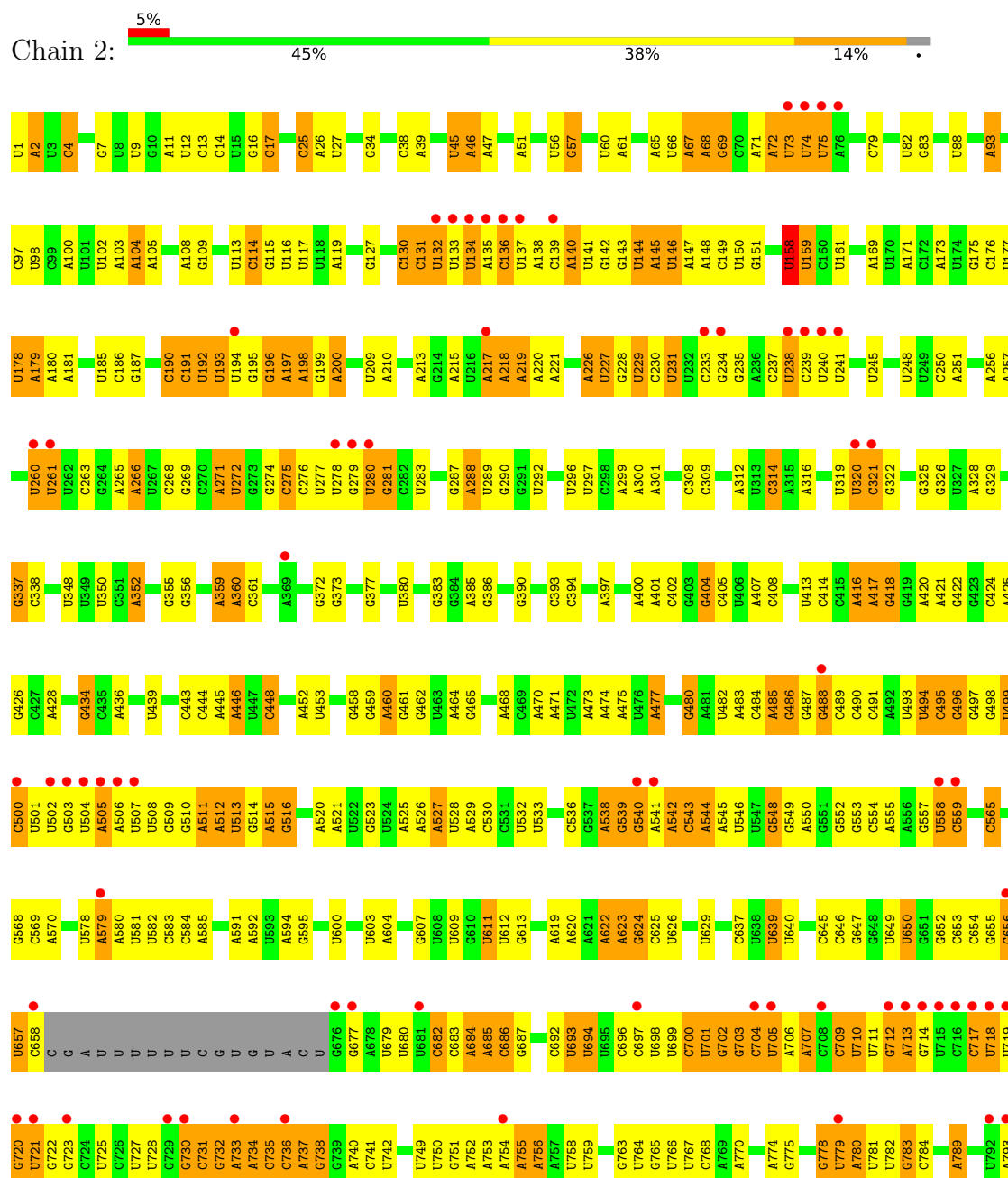


| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 88  | 1     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 33    | 26 | 1 | 6 |         |         |
| 88  | 5     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 33    | 26 | 1 | 6 |         |         |

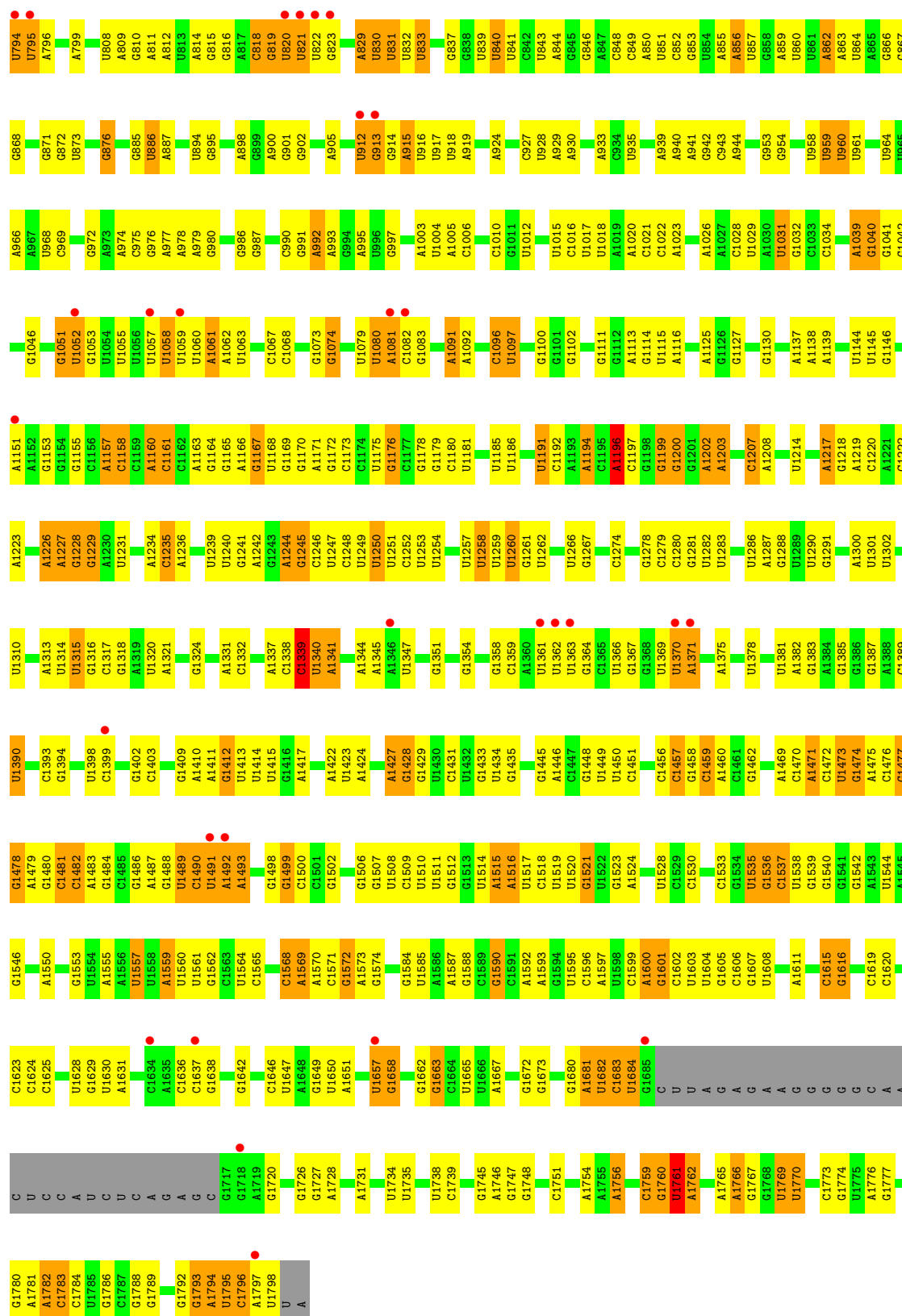
### 3 Residue-property plots

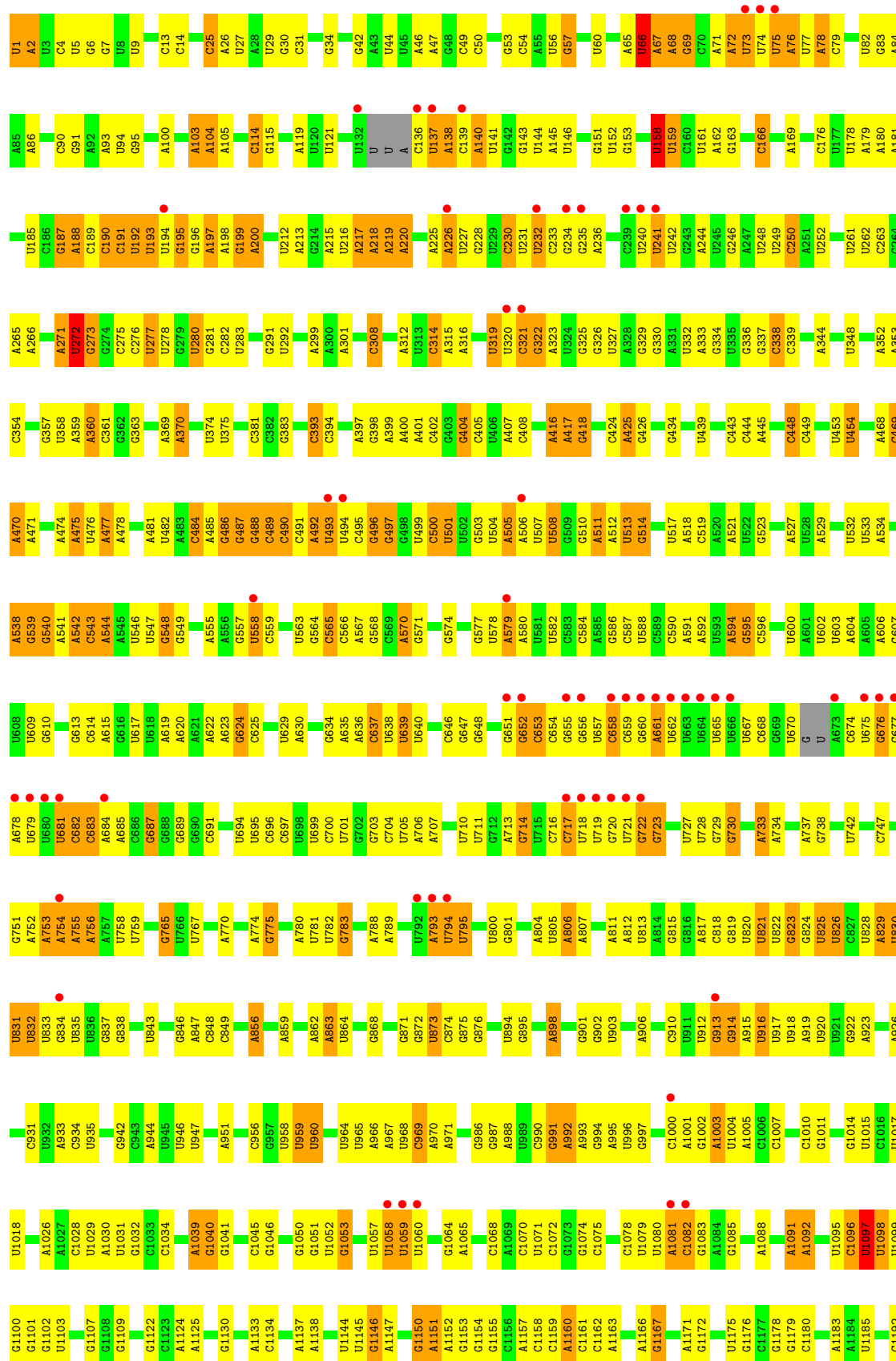
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

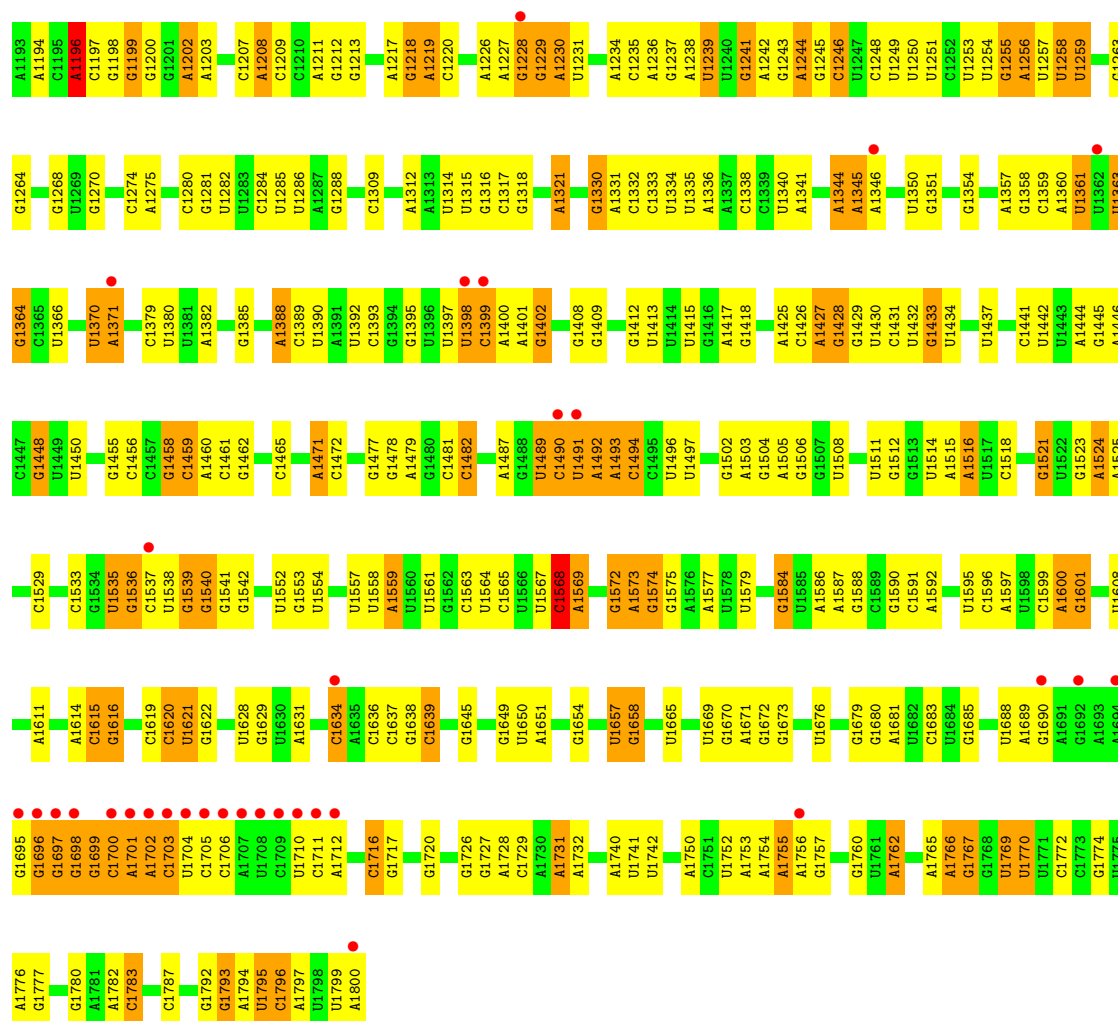
- Molecule 1: 18S ribosomal RNA



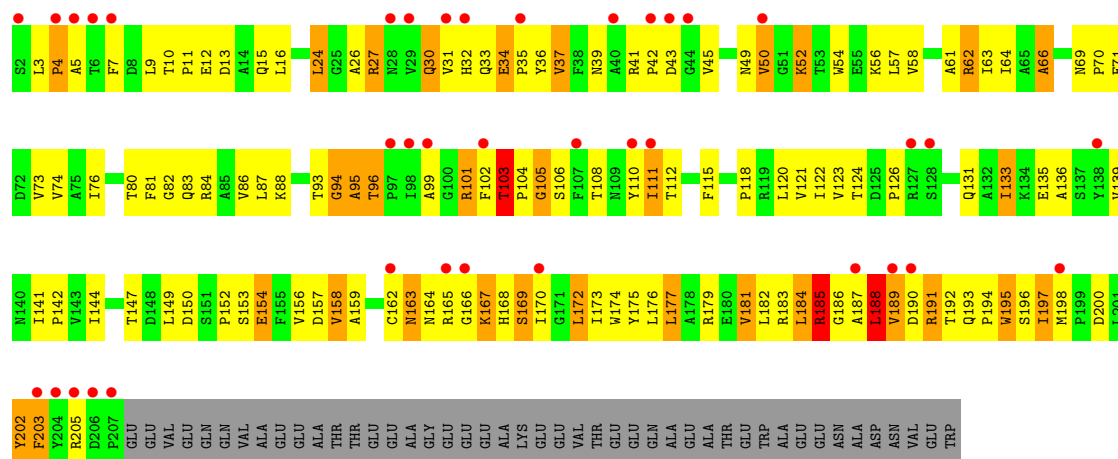




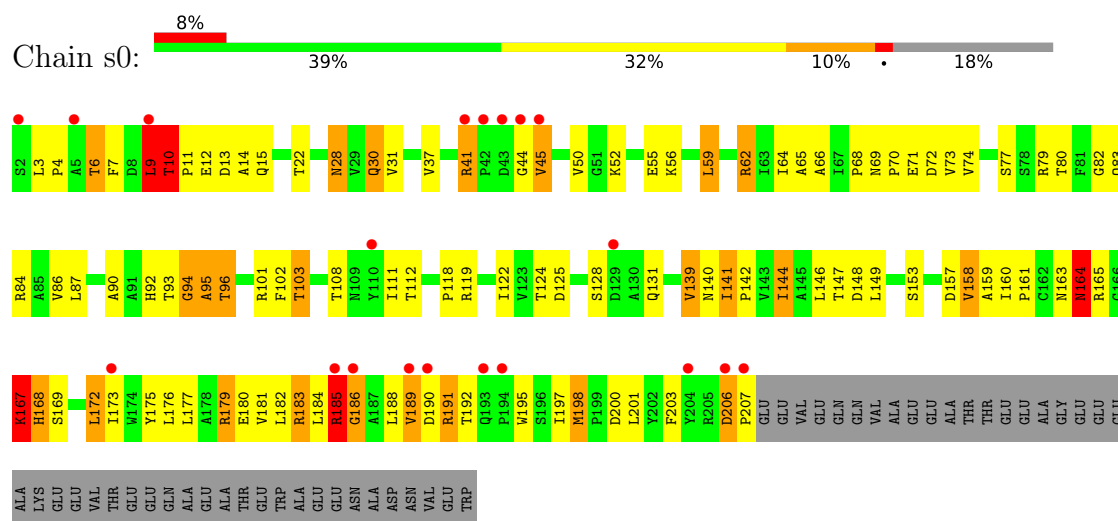




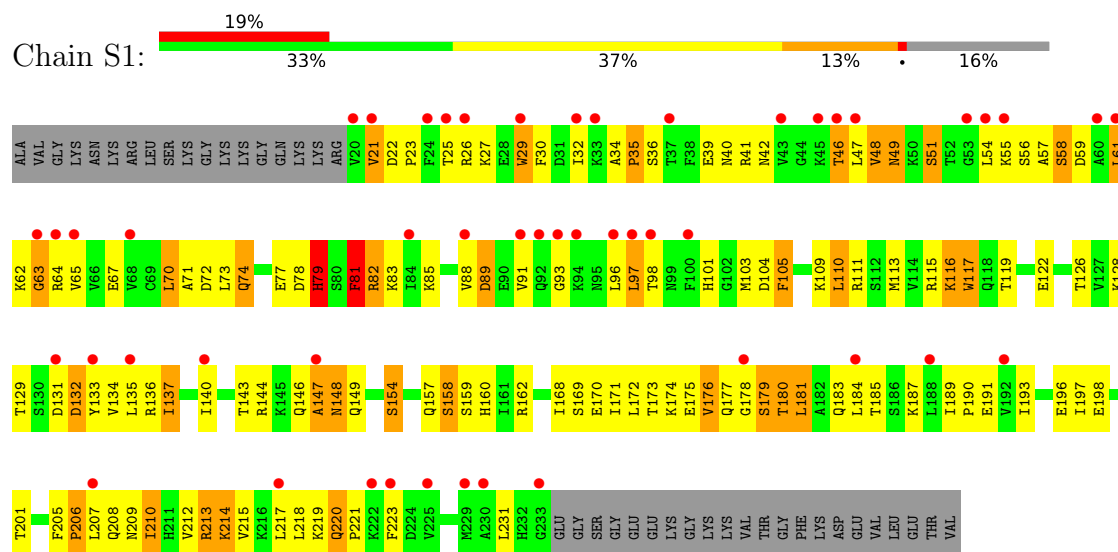
• Molecule 2: 40S ribosomal protein S0-A



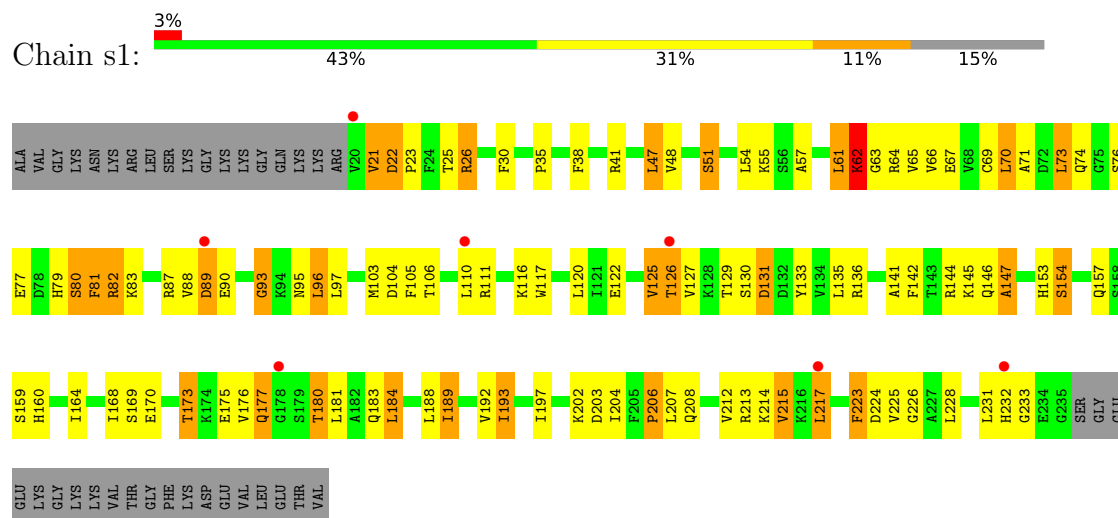
• Molecule 2: 40S ribosomal protein S0-A



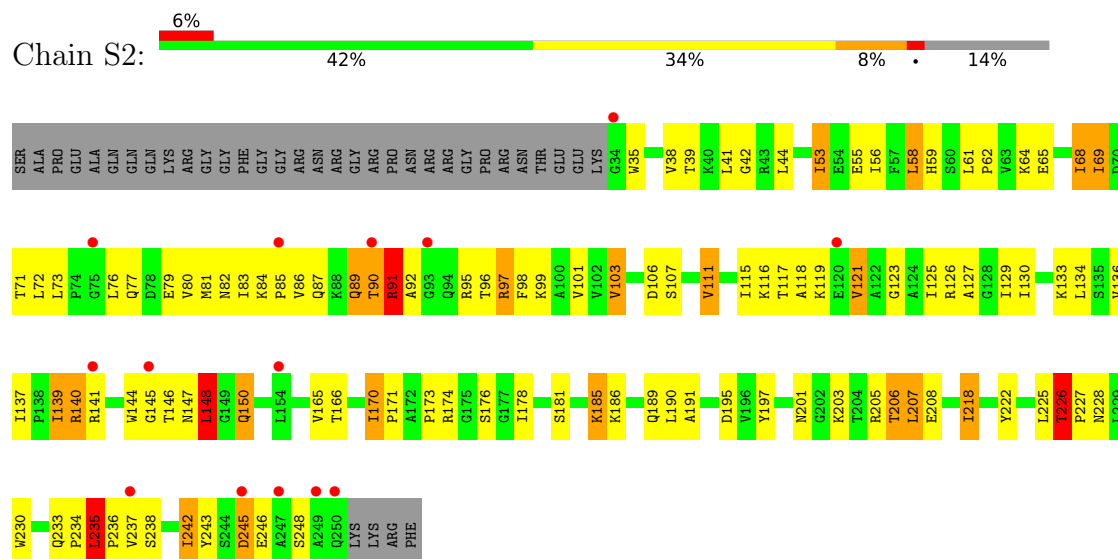
• Molecule 3: 40S ribosomal protein S1-A



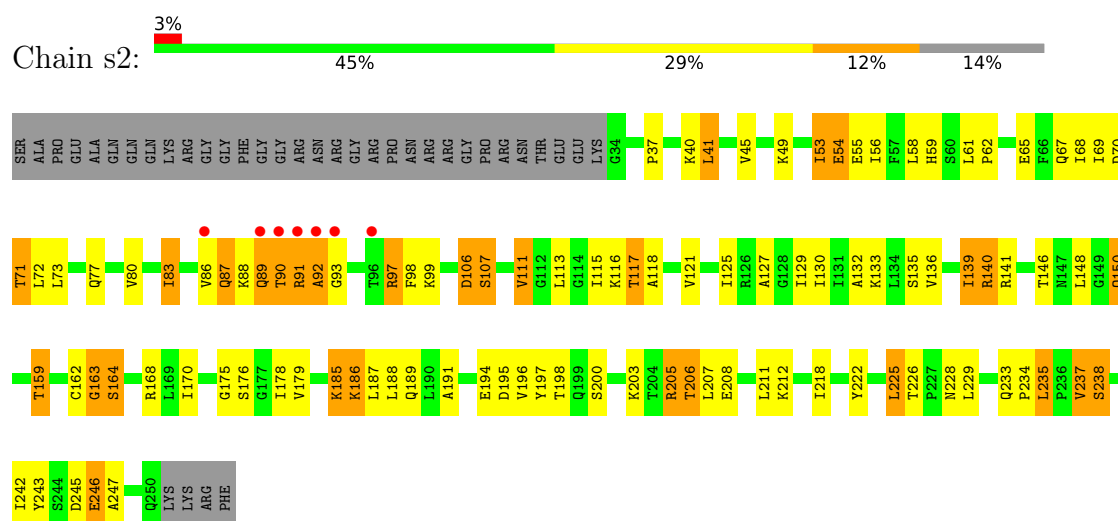
• Molecule 3: 40S ribosomal protein S1-A



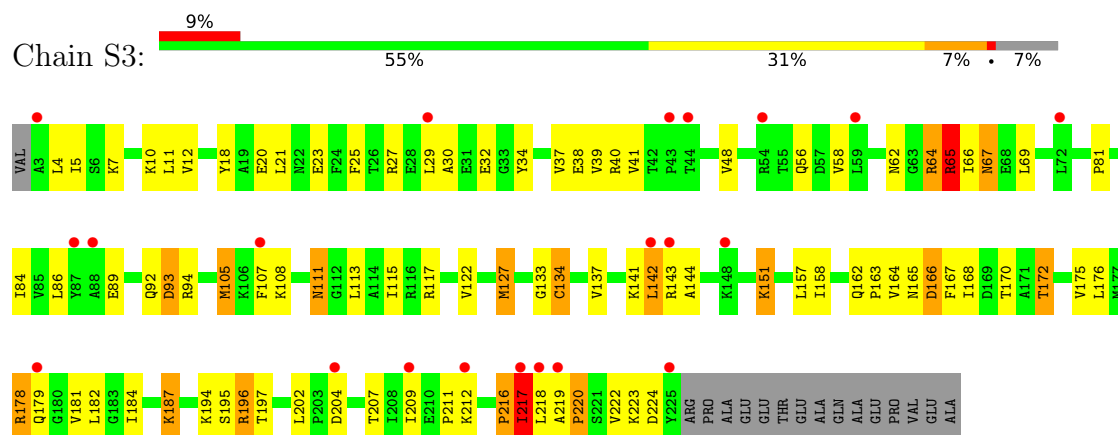
- Molecule 4: 40S ribosomal protein S2



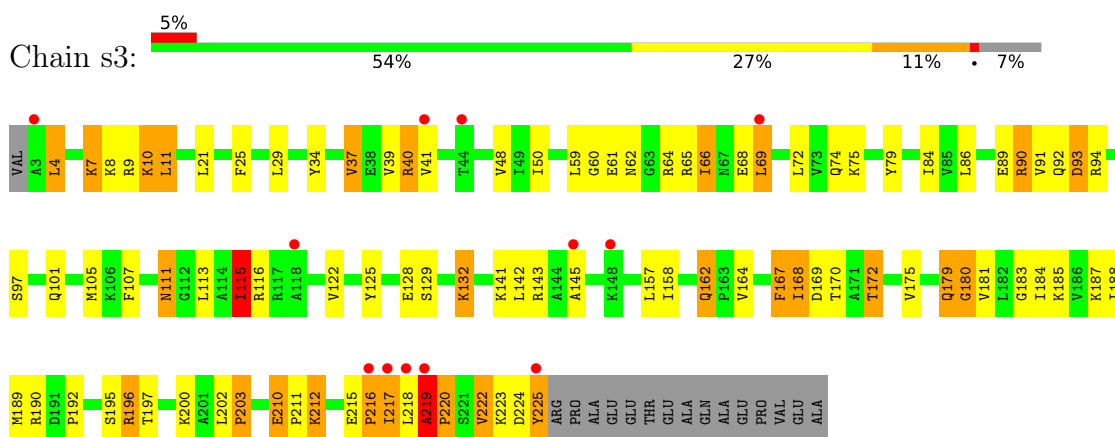
- Molecule 4: 40S ribosomal protein S2



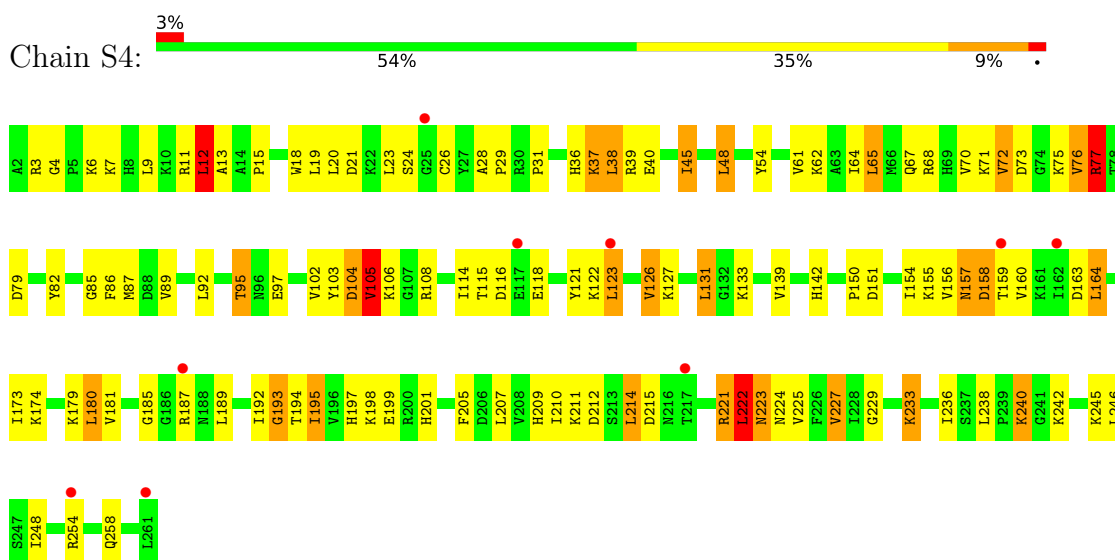
- Molecule 5: 40S ribosomal protein S3



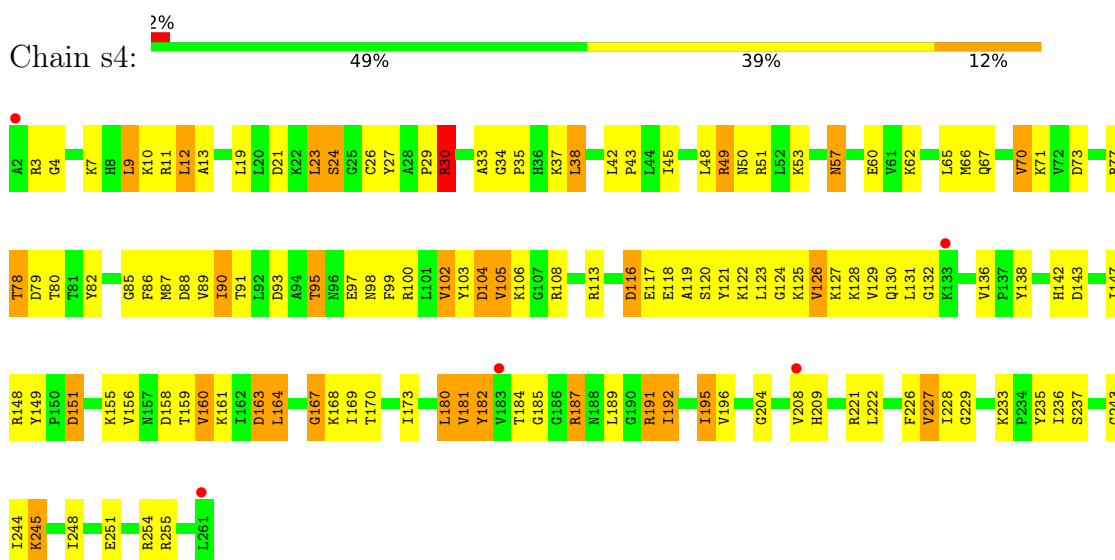
- Molecule 5: 40S ribosomal protein S3



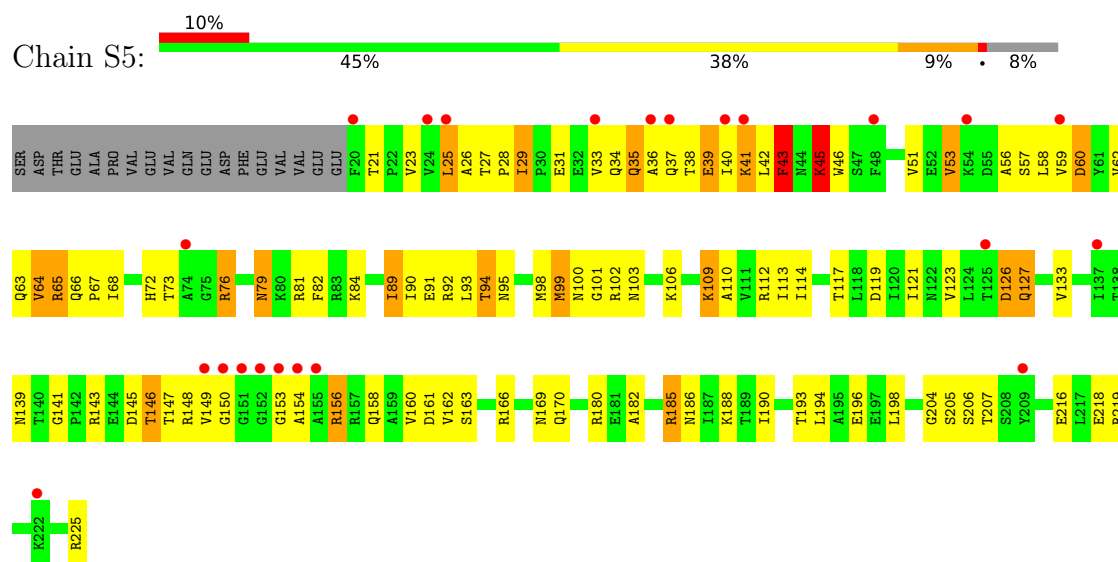
- Molecule 6: 40S ribosomal protein S4-A



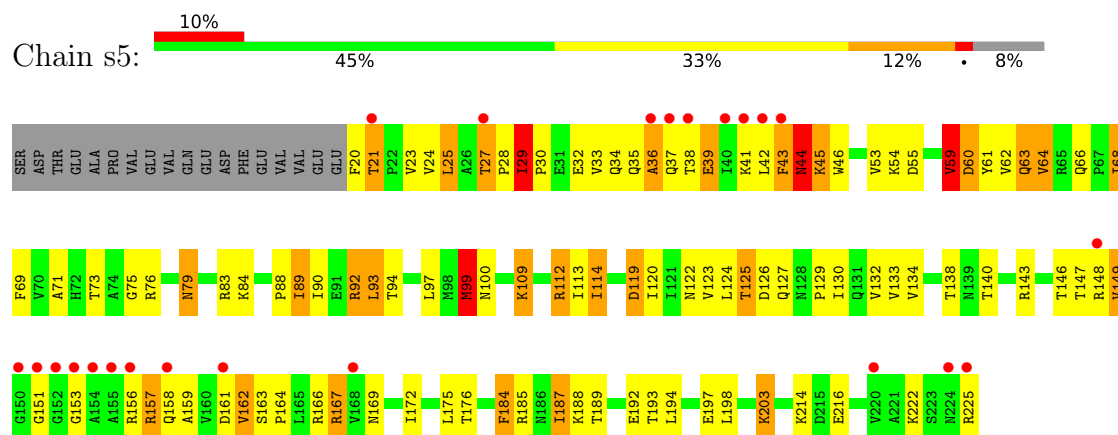
- Molecule 6: 40S ribosomal protein S4-A



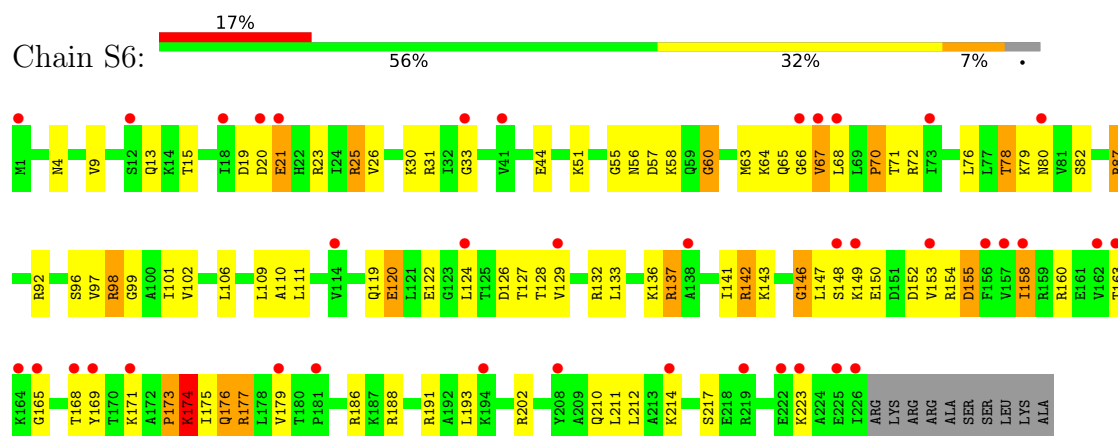
- Molecule 7: 40S ribosomal protein S5



• Molecule 7: 40S ribosomal protein S5

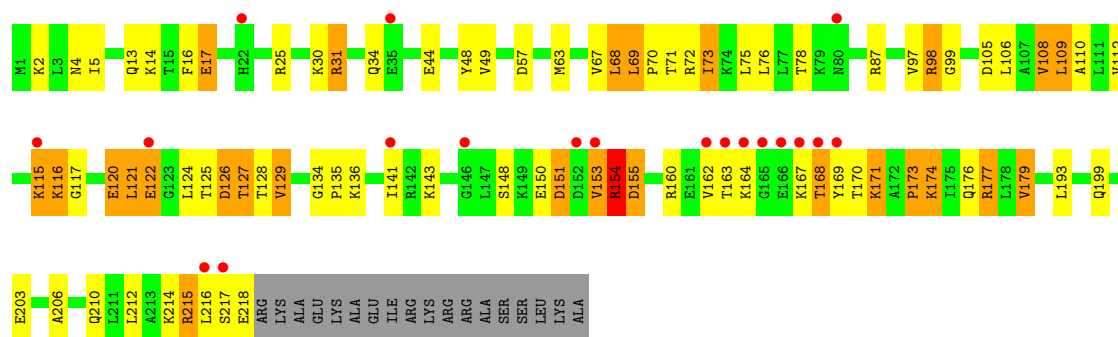


• Molecule 8: 40S ribosomal protein S6-A

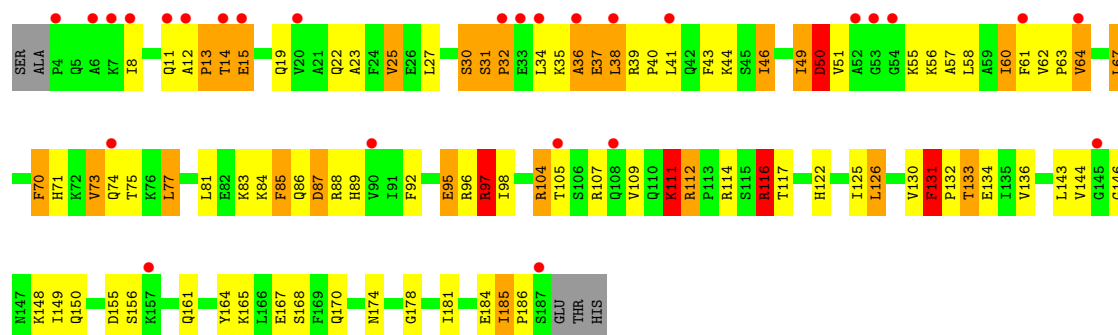


• Molecule 8: 40S ribosomal protein S6-A

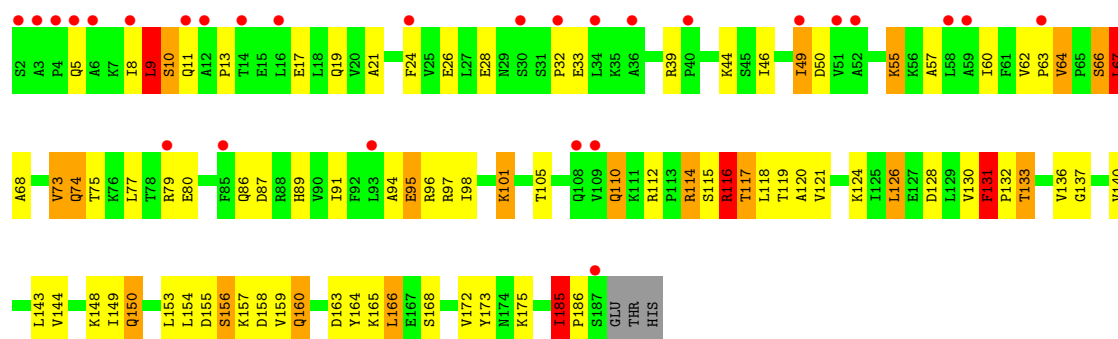




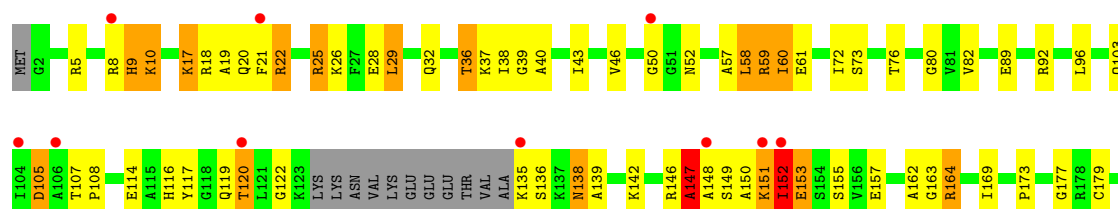
• Molecule 9: 40S ribosomal protein S7-A



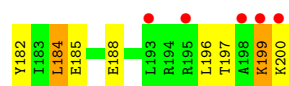
• Molecule 9: 40S ribosomal protein S7-A



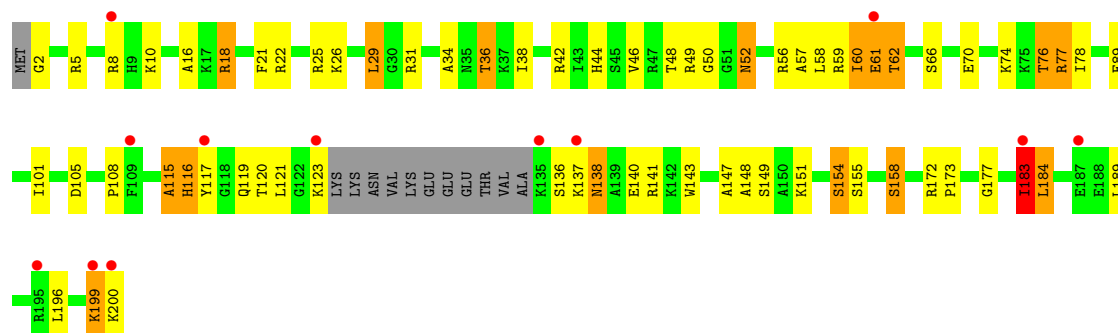
• Molecule 10: 40S ribosomal protein S8-A



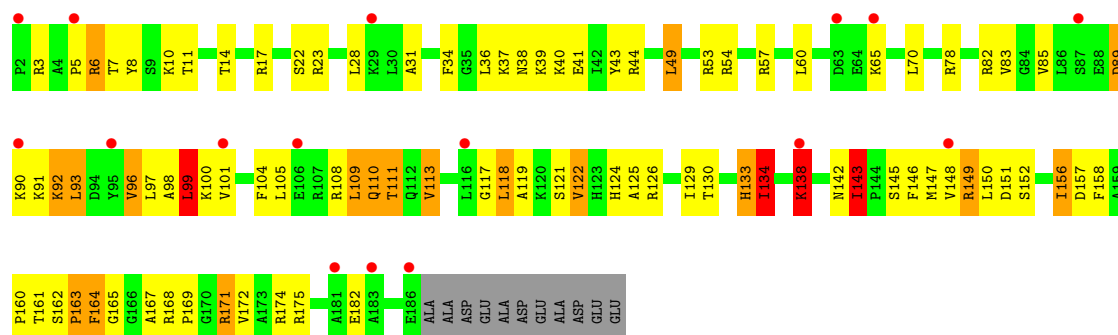




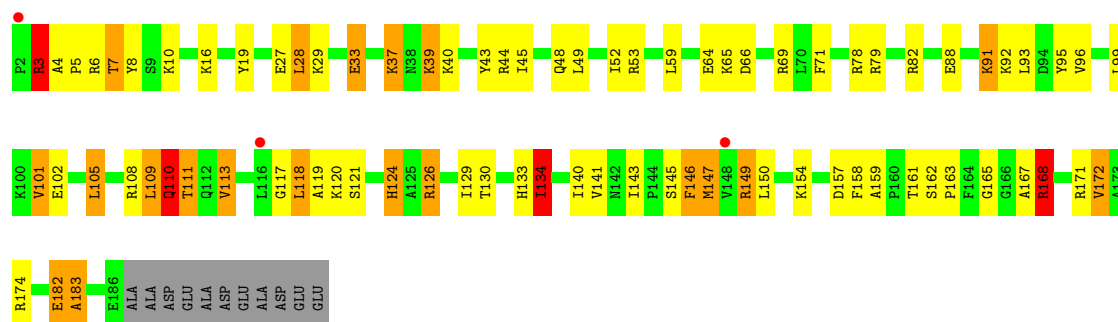
• Molecule 10: 40S ribosomal protein S8-A



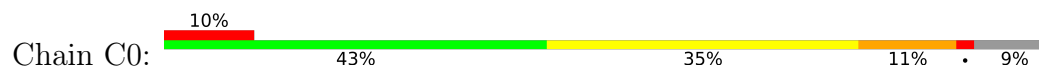
• Molecule 11: 40S ribosomal protein S9-A

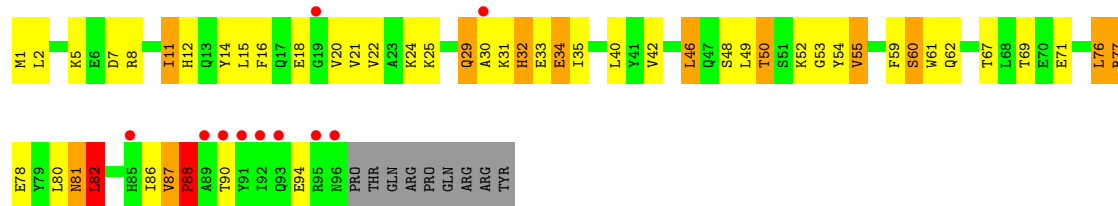


• Molecule 11: 40S ribosomal protein S9-A

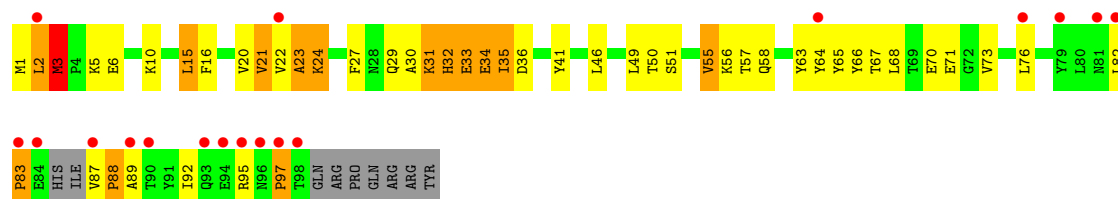


• Molecule 12: 40S ribosomal protein S10-A

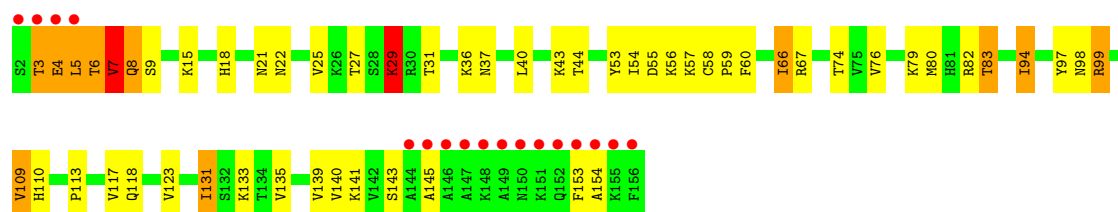




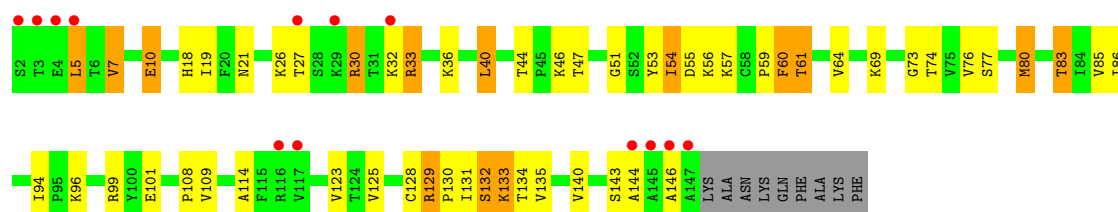
• Molecule 12: 40S ribosomal protein S10-A



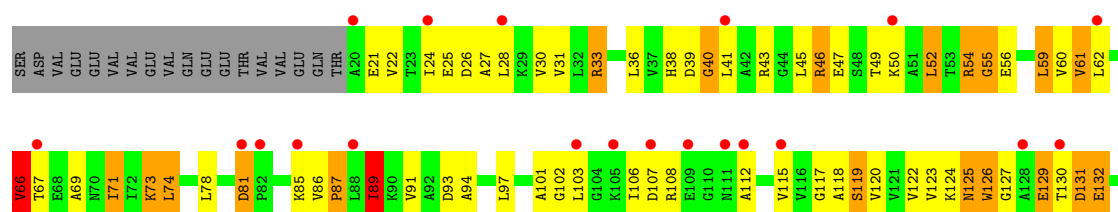
• Molecule 13: 40S ribosomal protein S11-A



• Molecule 13: 40S ribosomal protein S11-A



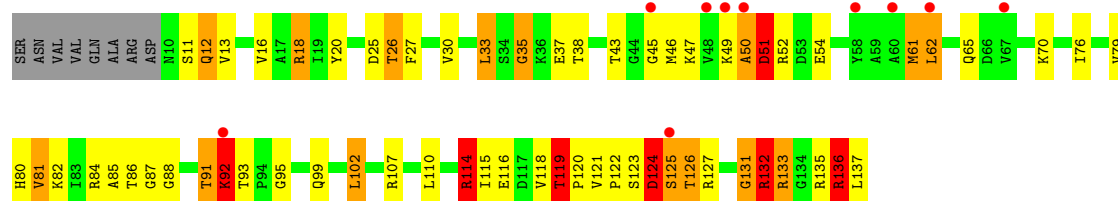
• Molecule 14: 40S ribosomal protein S12





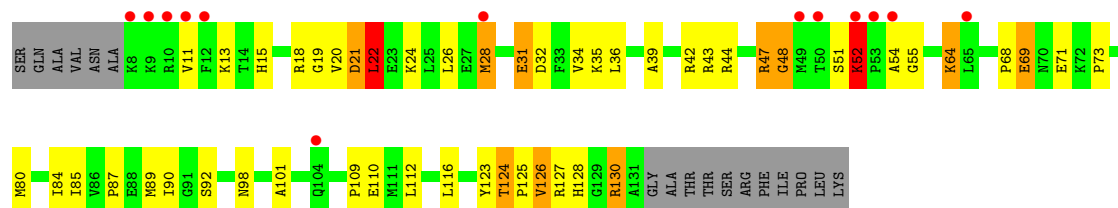
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 



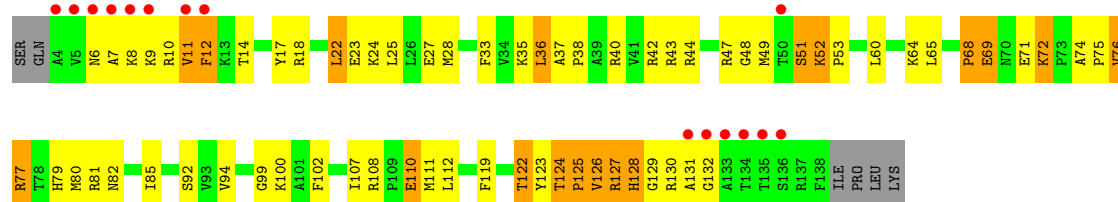
- Molecule 17: 40S ribosomal protein S15

Chain C5: 



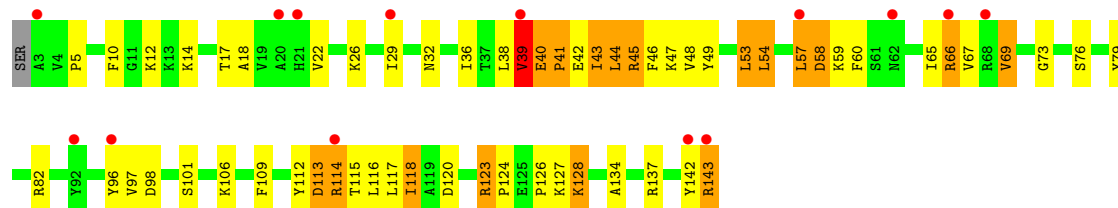
- Molecule 17: 40S ribosomal protein S15

Chain c5: 



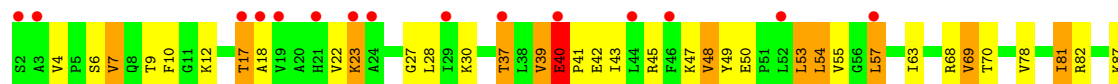
- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 



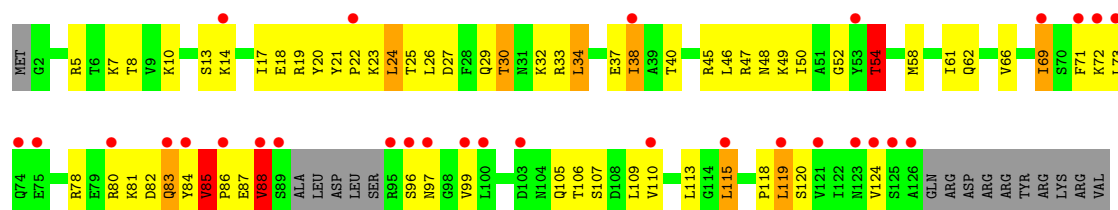
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 





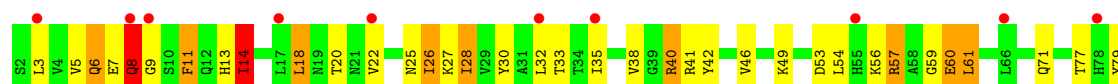
• Molecule 19: 40S ribosomal protein S17-A



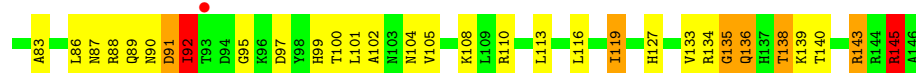
• Molecule 19: 40S ribosomal protein S17-A



• Molecule 20: 40S ribosomal protein S18-A

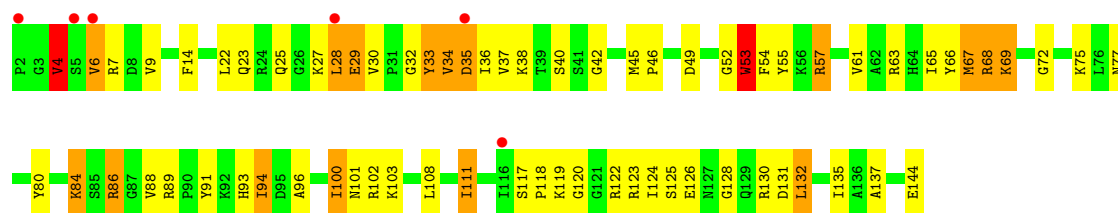


• Molecule 20: 40S ribosomal protein S18-A

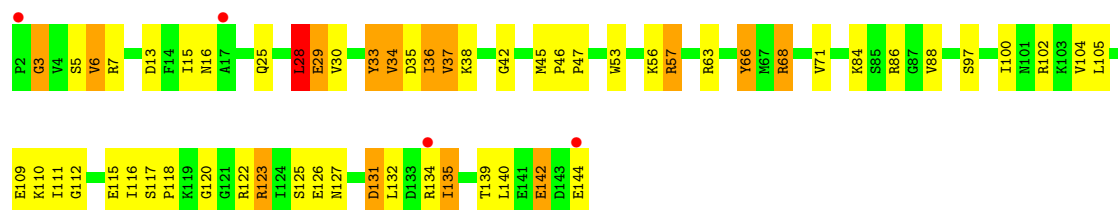


• Molecule 21: 40S ribosomal protein S19-A

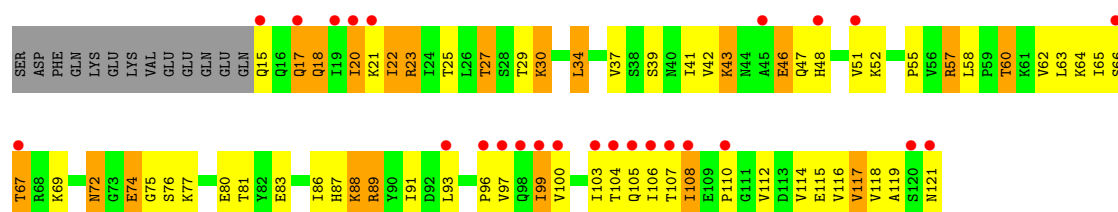




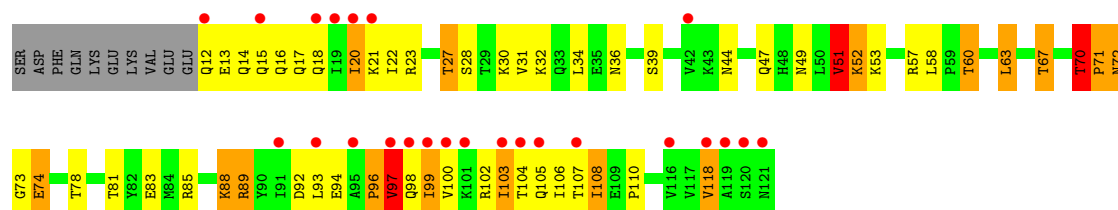
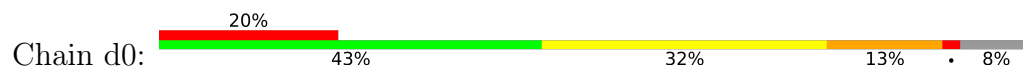
• Molecule 21: 40S ribosomal protein S19-A



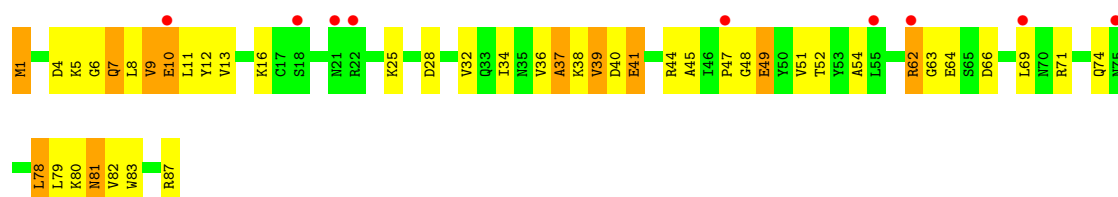
• Molecule 22: 40S ribosomal protein S20



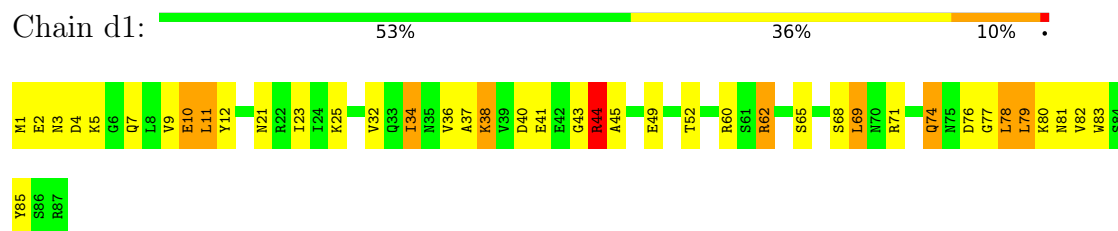
• Molecule 22: 40S ribosomal protein S20



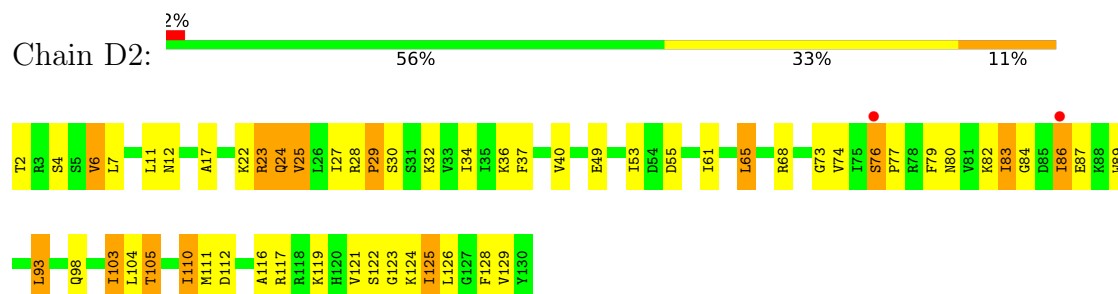
• Molecule 23: 40S ribosomal protein S21-A



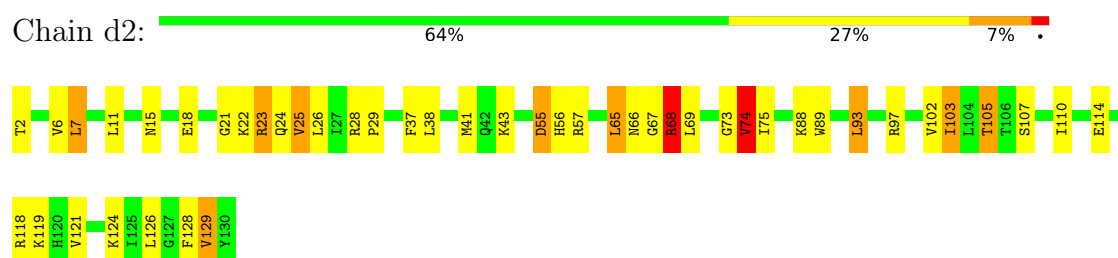
- Molecule 23: 40S ribosomal protein S21-A



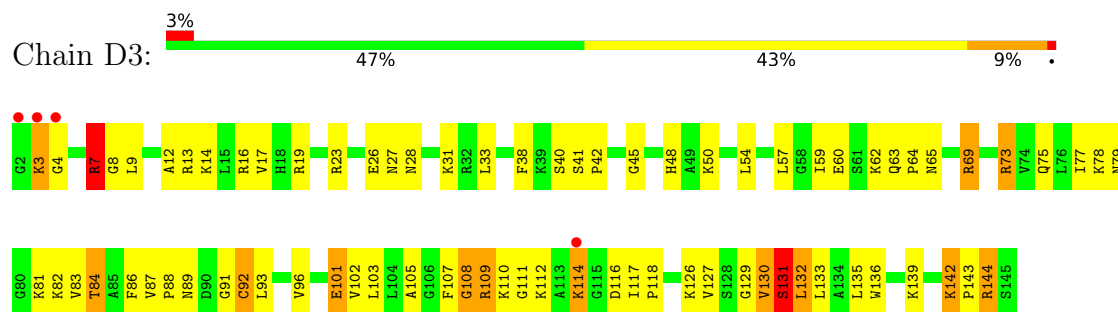
- Molecule 24: 40S ribosomal protein S22-A



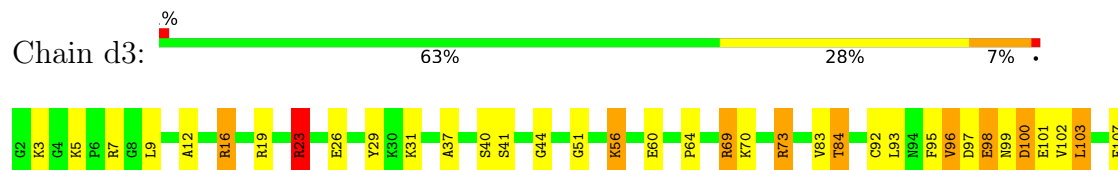
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 25: 40S ribosomal protein S23-A



- Molecule 25: 40S ribosomal protein S23-A

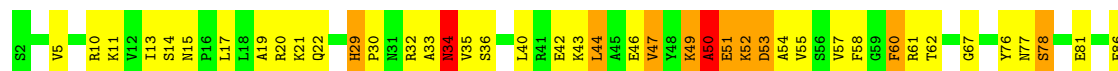




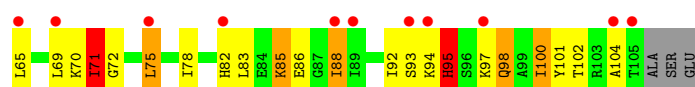
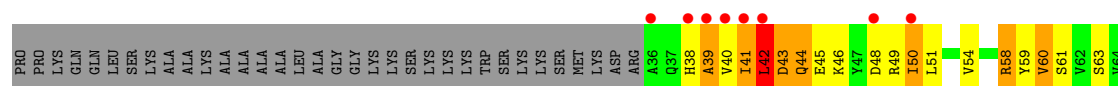
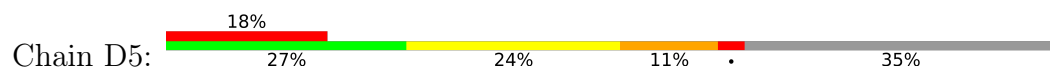
- Molecule 26: 40S ribosomal protein S24-A



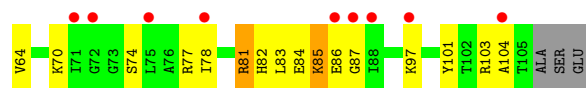
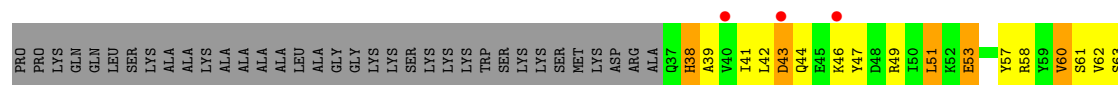
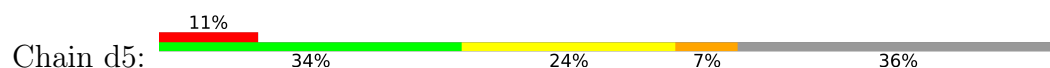
- Molecule 26: 40S ribosomal protein S24-A



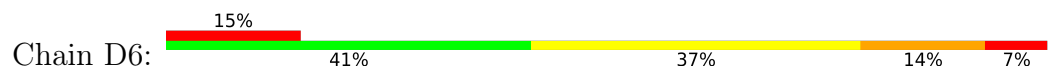
- Molecule 27: 40S ribosomal protein S25-A



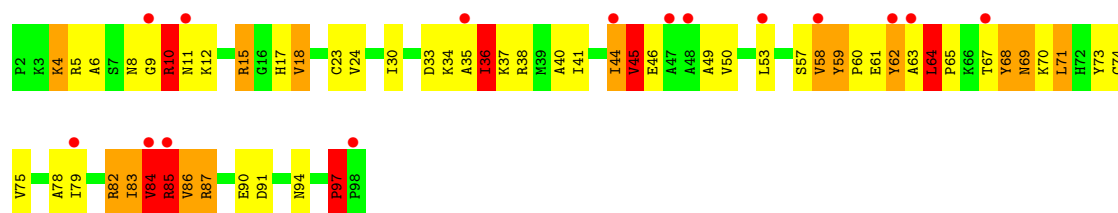
- Molecule 27: 40S ribosomal protein S25-A



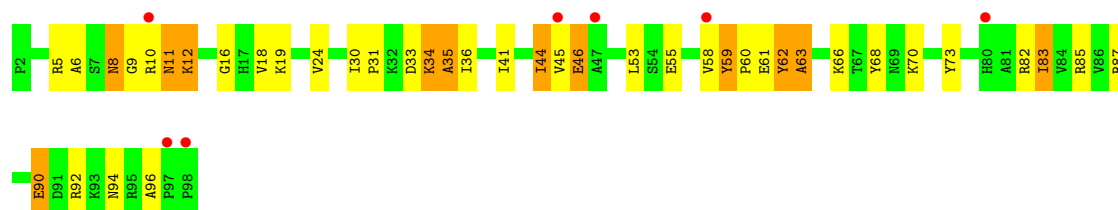
- Molecule 28: 40S ribosomal protein S26-B



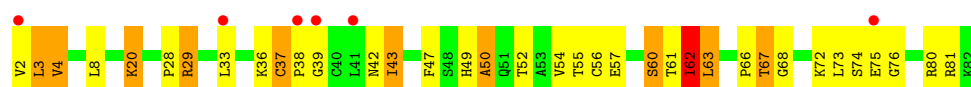




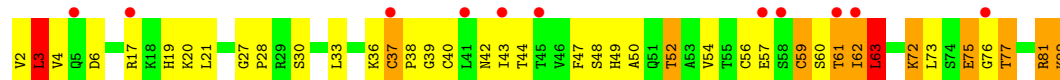
• Molecule 28: 40S ribosomal protein S26-B



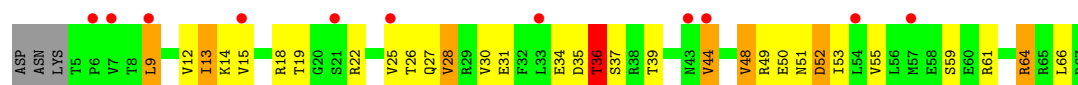
• Molecule 29: 40S ribosomal protein S27-A



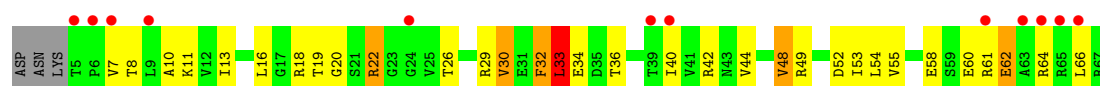
• Molecule 29: 40S ribosomal protein S27-A



• Molecule 30: 40S ribosomal protein S28-A



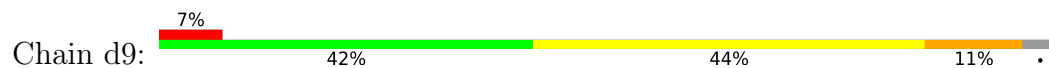
• Molecule 30: 40S ribosomal protein S28-A



• Molecule 31: 40S ribosomal protein S29-A



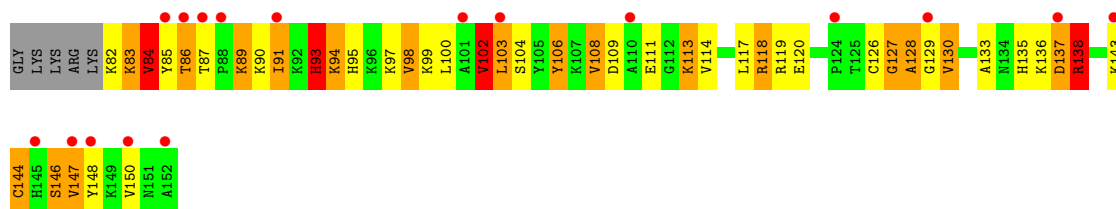
- Molecule 31: 40S ribosomal protein S29-A



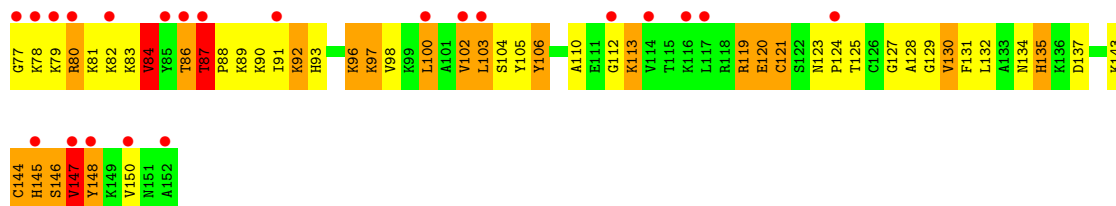
- Molecule 32: 40S ribosomal protein S30-A



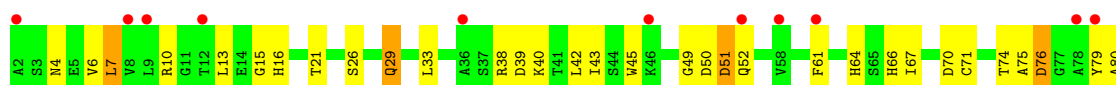
- Molecule 33: Ubiquitin-40S ribosomal protein S31

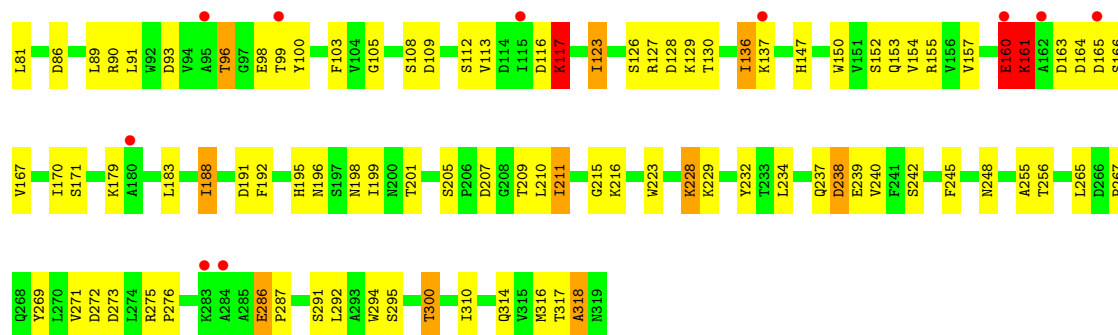


- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

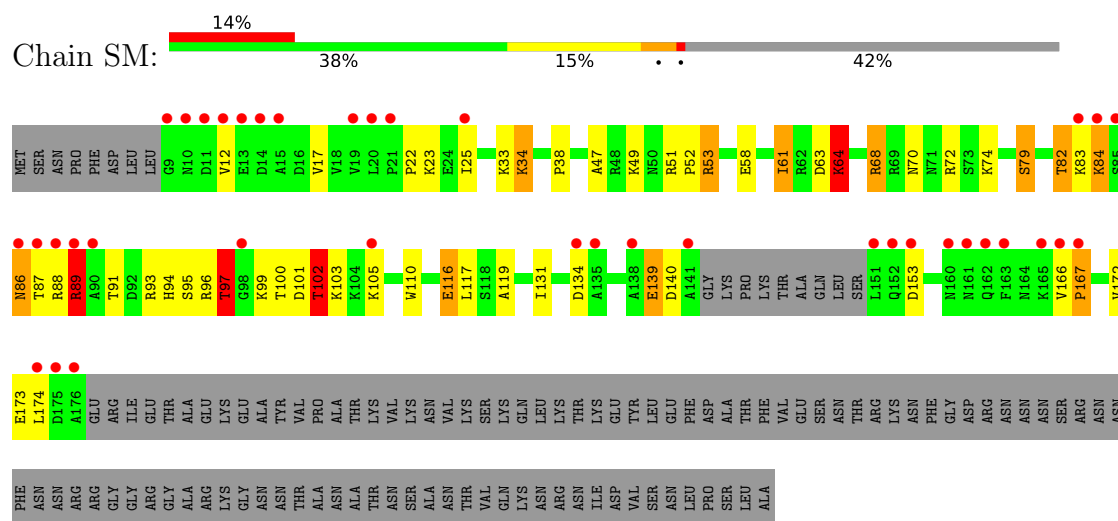




- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



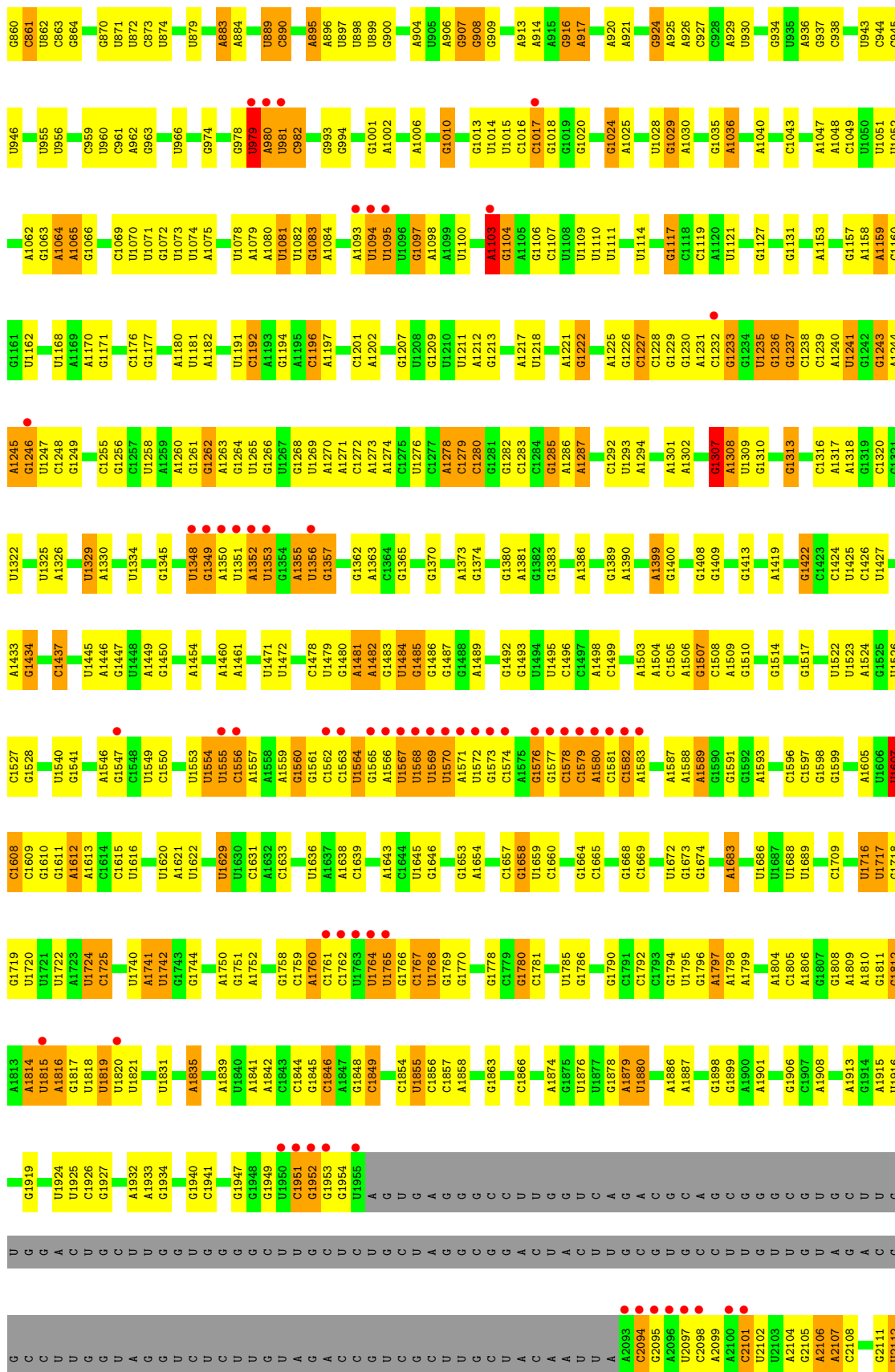
- Molecule 35: Suppressor protein STM1

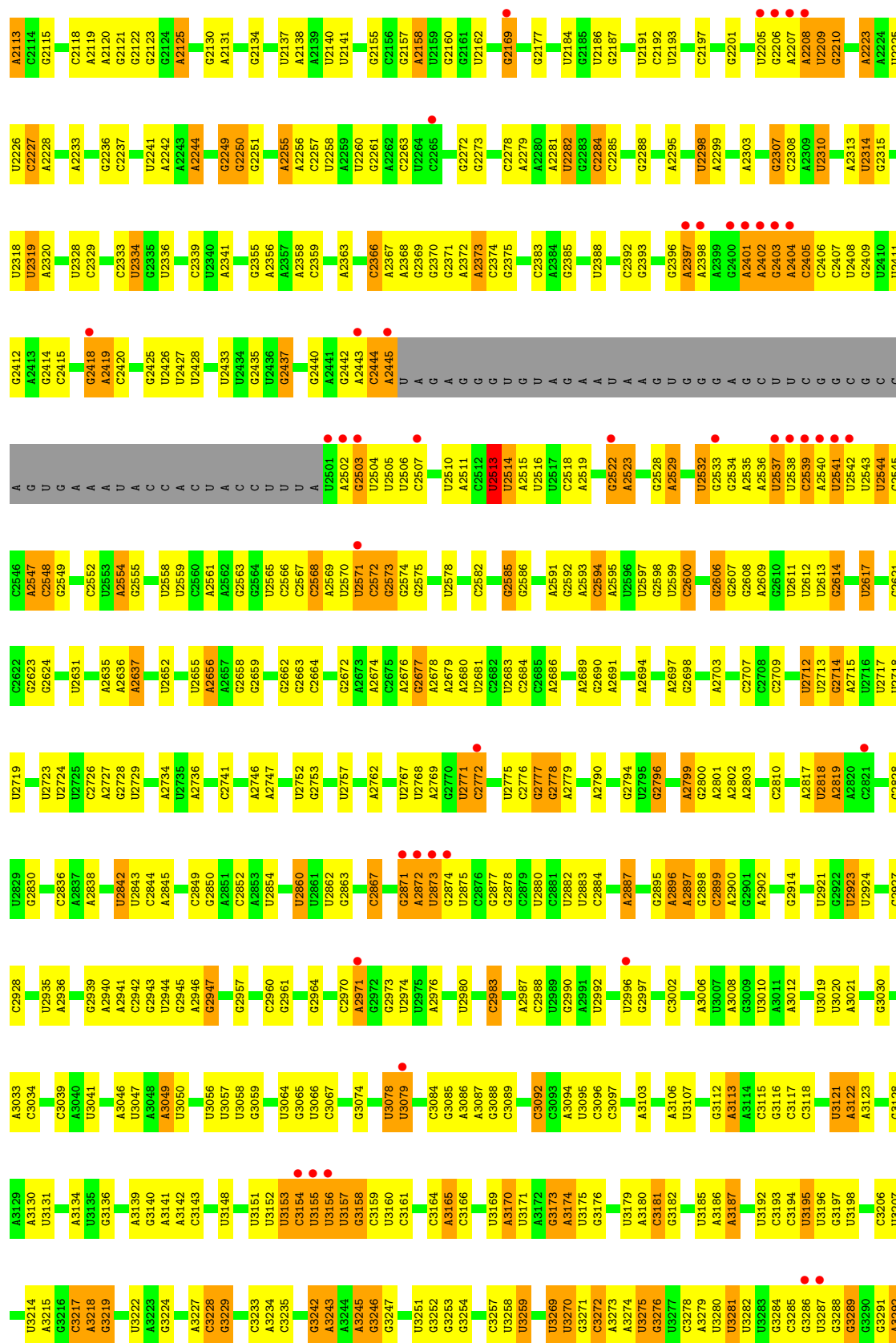


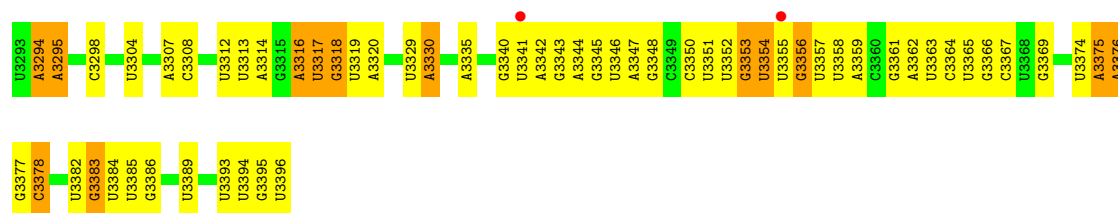
- Molecule 35: Suppressor protein STM1



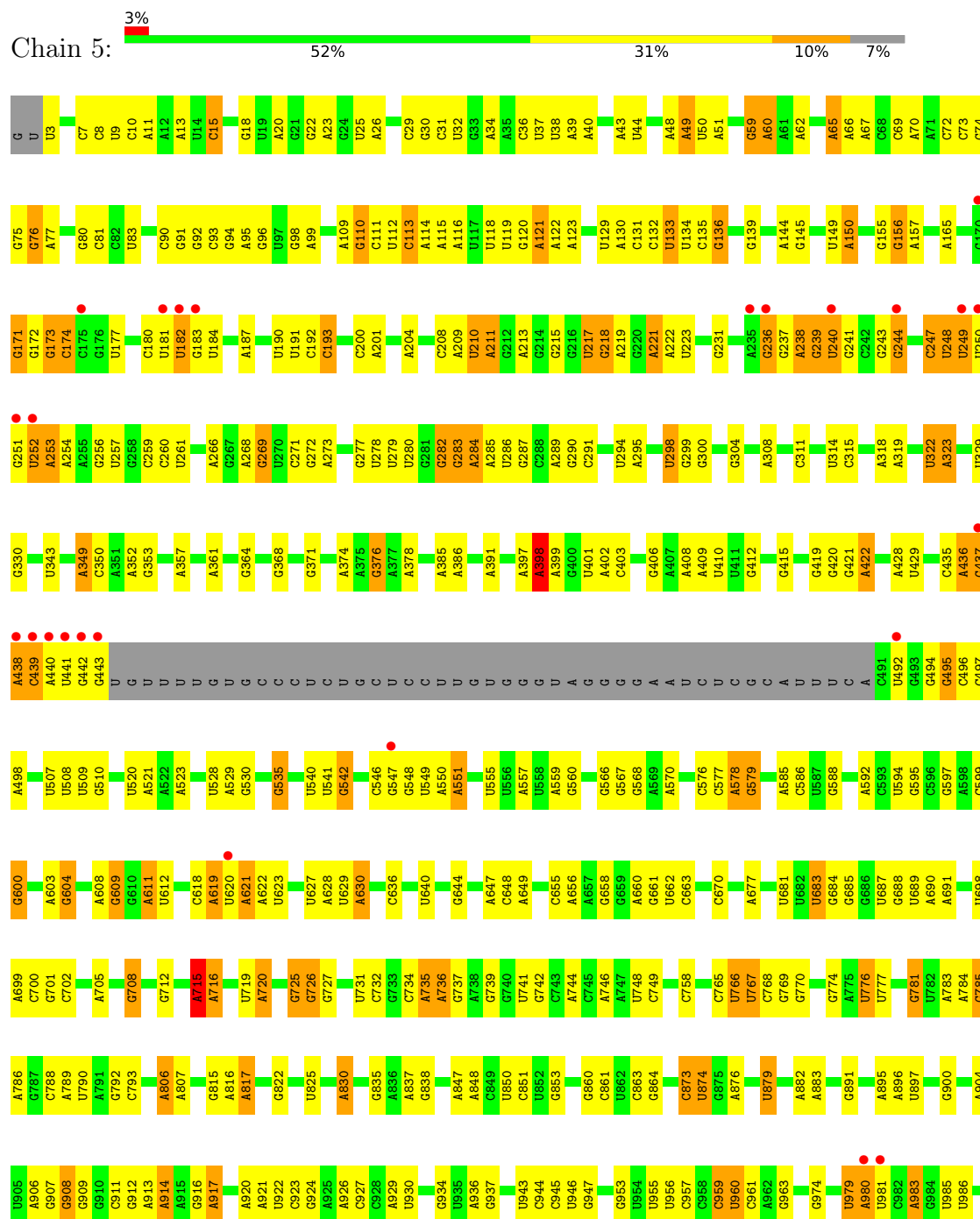






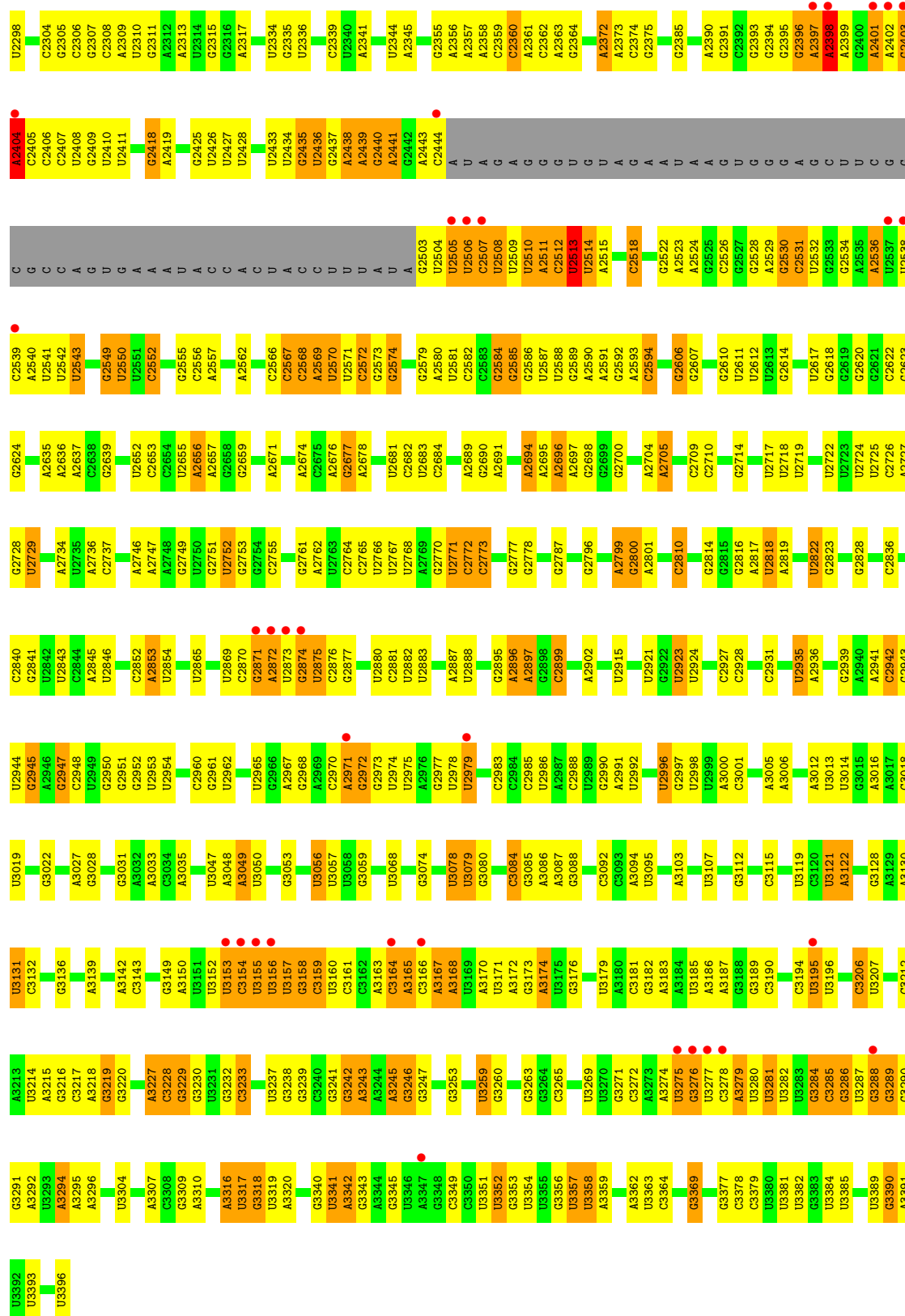


• Molecule 36: 25S ribosomal RNA



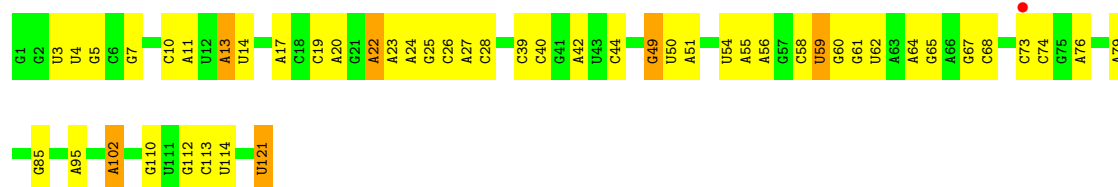
[illegible]



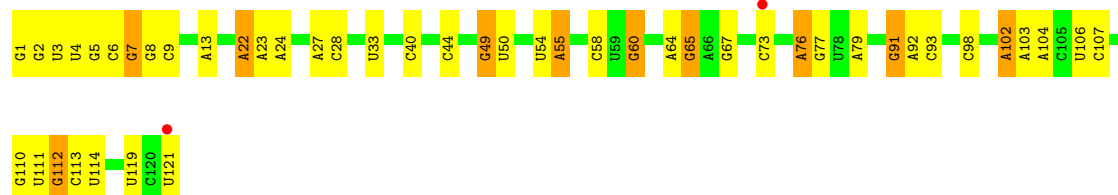


- Molecule 37: 5S ribosomal RNA

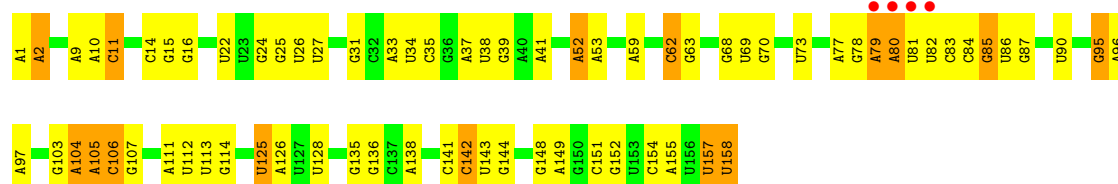




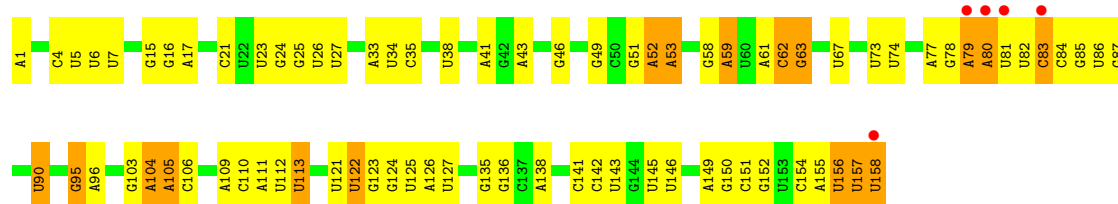
• Molecule 37: 5S ribosomal RNA



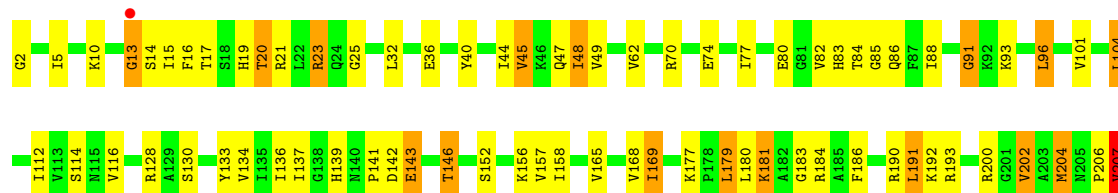
• Molecule 38: 5.8S ribosomal RNA

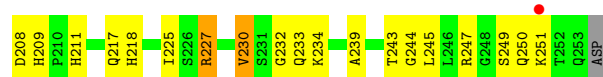


• Molecule 38: 5.8S ribosomal RNA

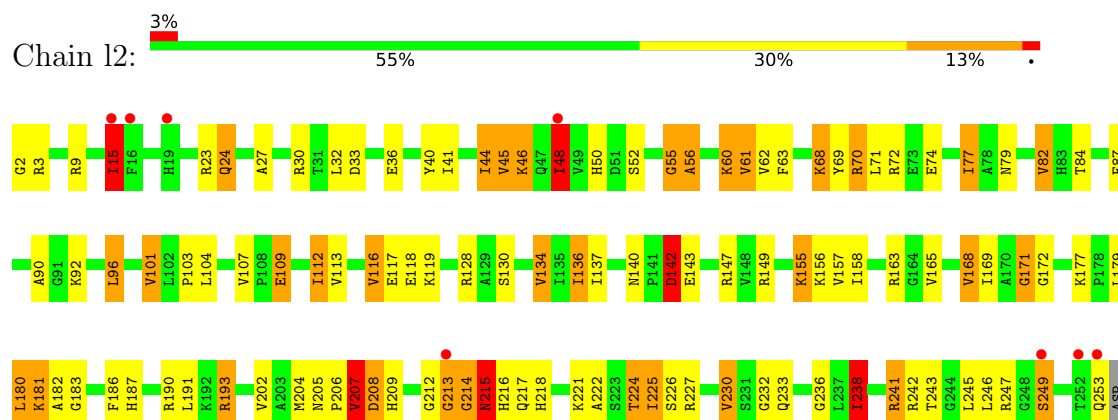


• Molecule 39: 60S ribosomal protein L2-A

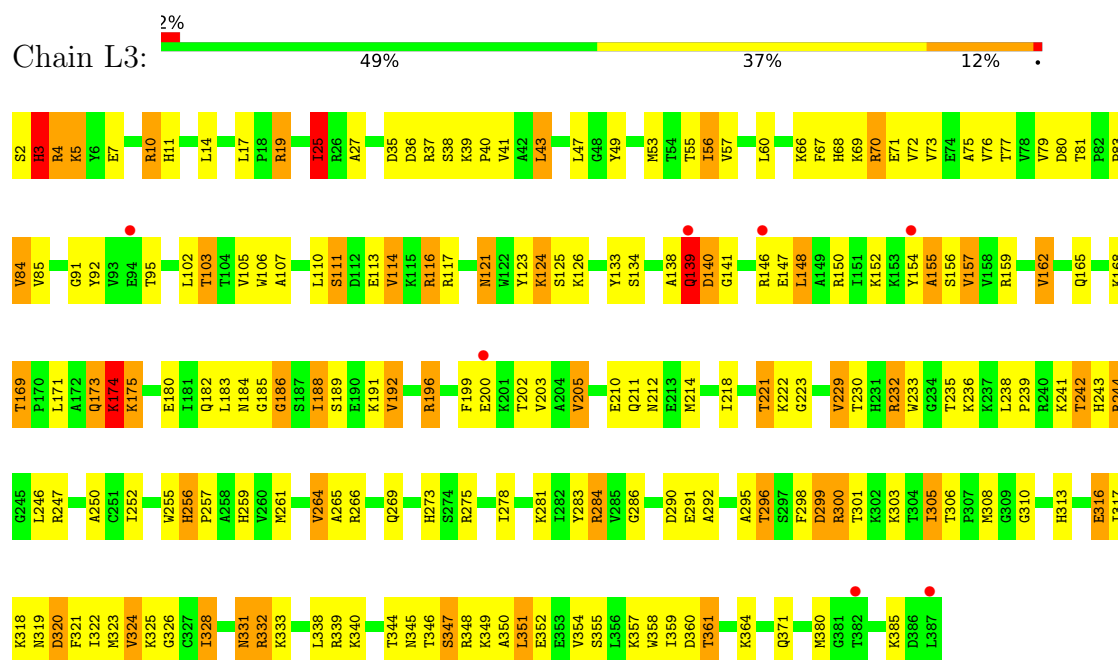




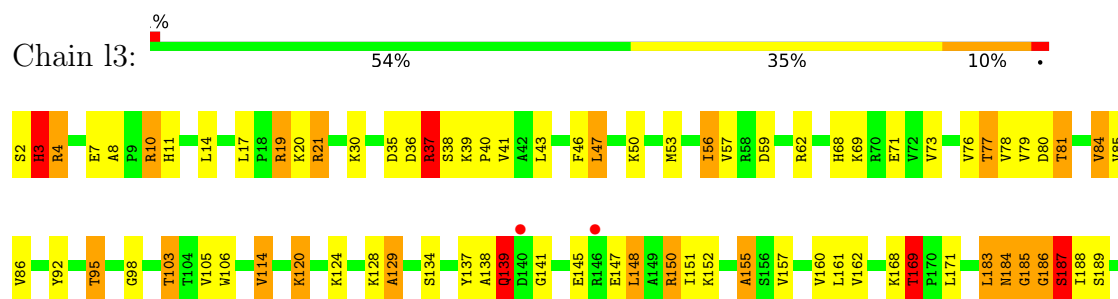
- Molecule 39: 60S ribosomal protein L2-A



- Molecule 40: 60S ribosomal protein L3

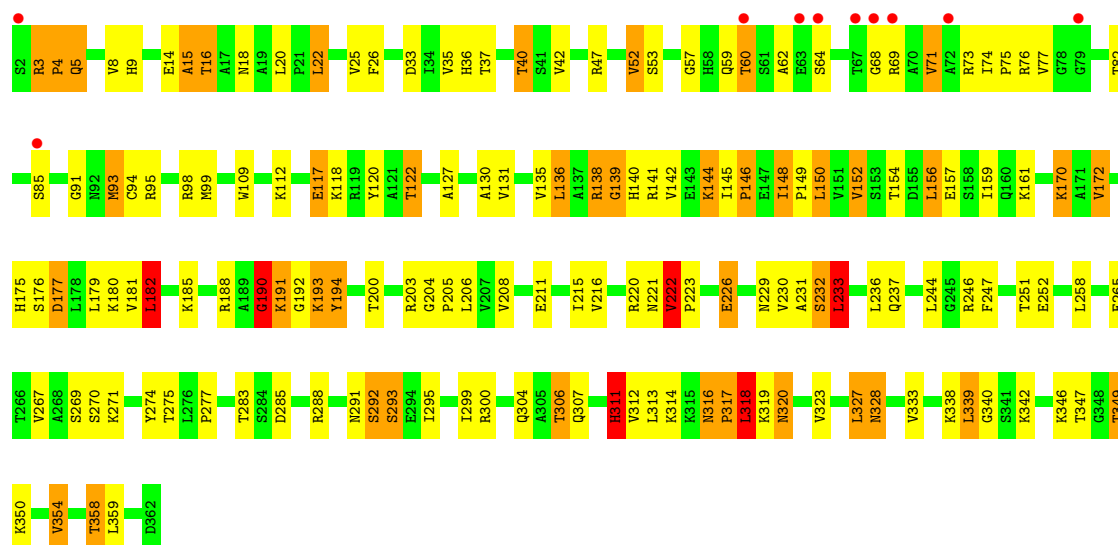


- Molecule 40: 60S ribosomal protein L3

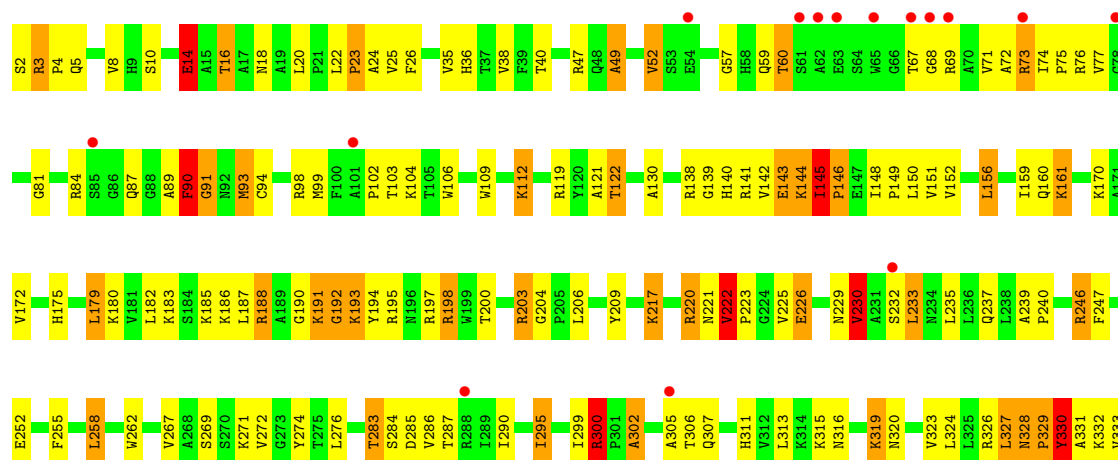




• Molecule 41: 60S ribosomal protein L4-A

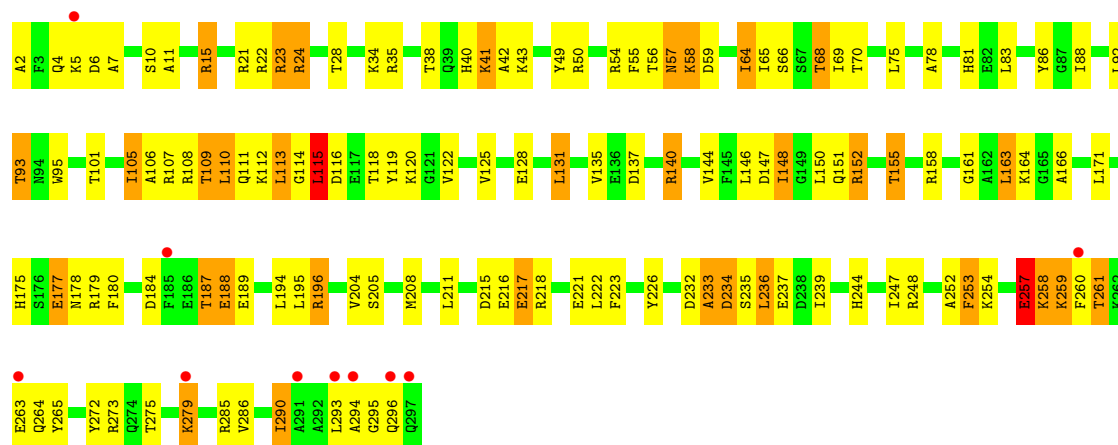


• Molecule 41: 60S ribosomal protein L4-A

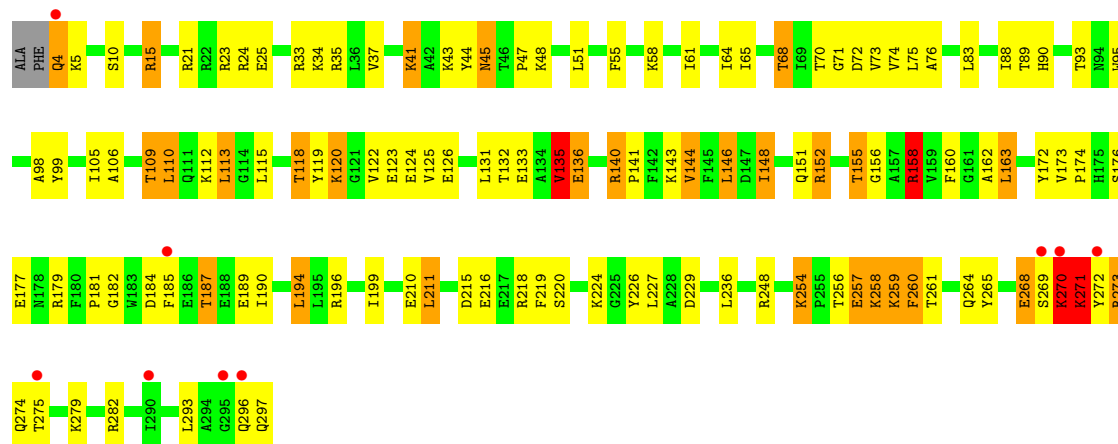




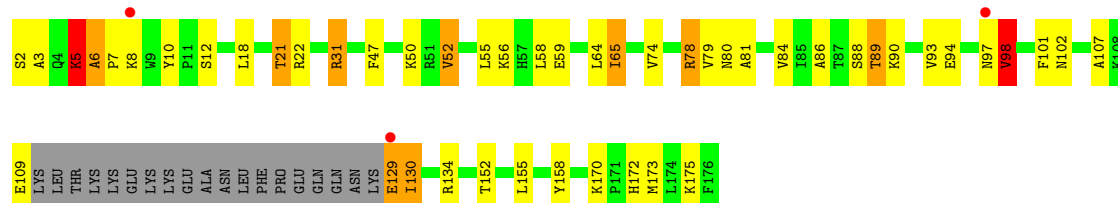
• Molecule 42: 60S ribosomal protein L5



• Molecule 42: 60S ribosomal protein L5

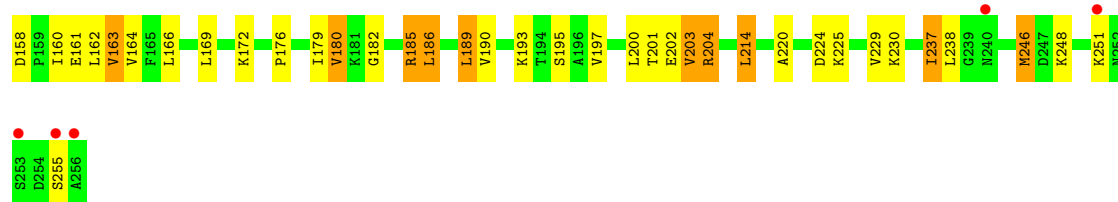


• Molecule 43: 60S ribosomal protein L6-A

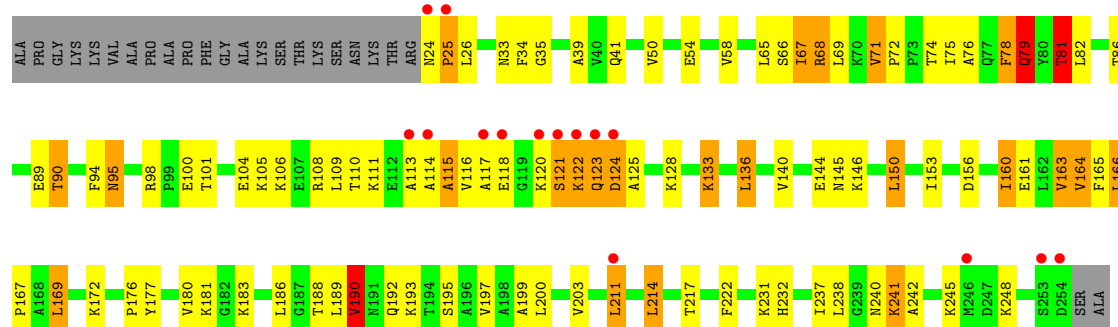


• Molecule 43: 60S ribosomal protein L6-A

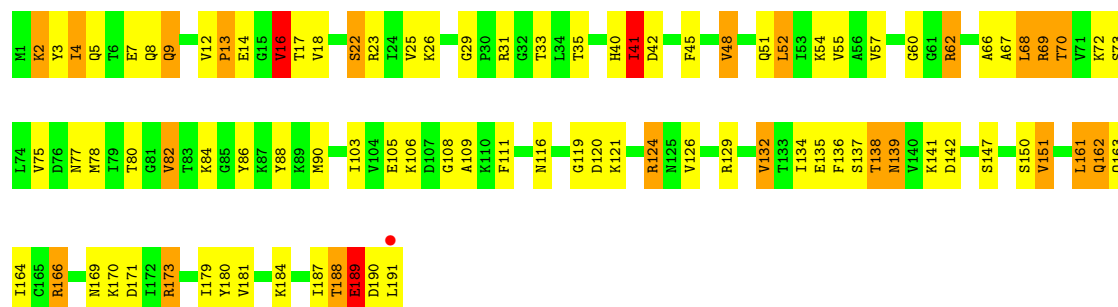




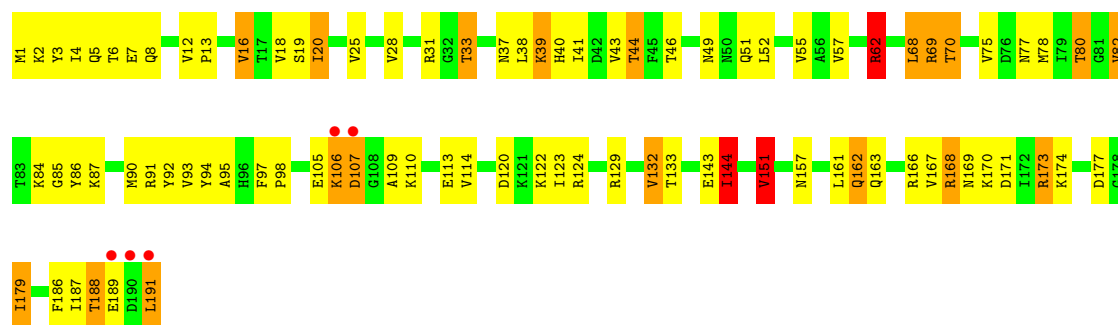
• Molecule 45: 60S ribosomal protein L8-A



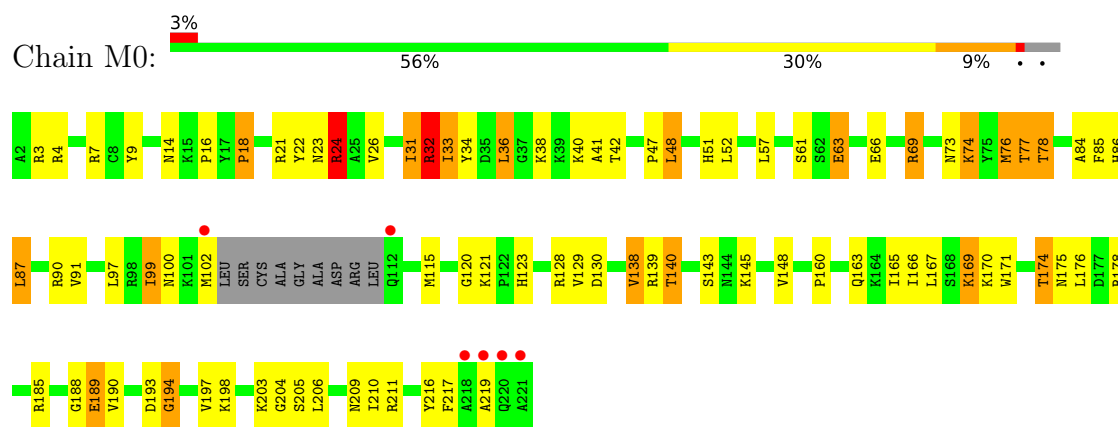
• Molecule 46: 60S ribosomal protein L9-A



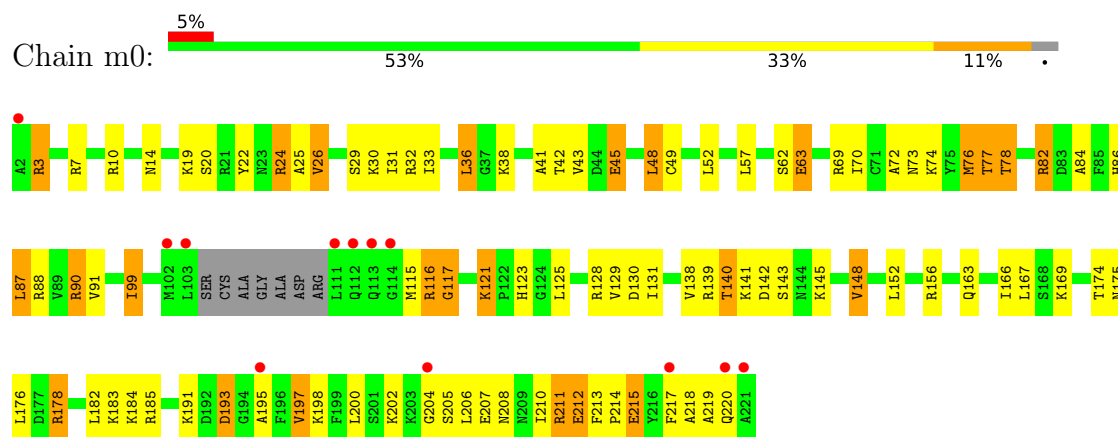
• Molecule 46: 60S ribosomal protein L9-A



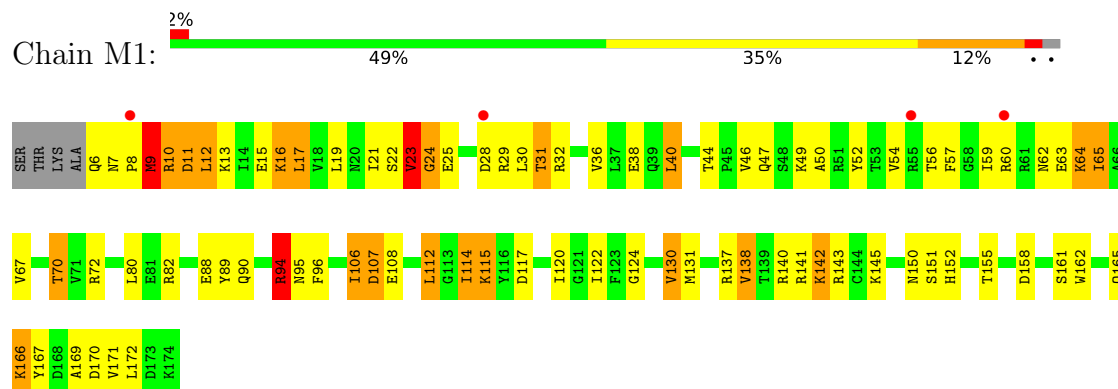
• Molecule 47: 60S ribosomal protein L10



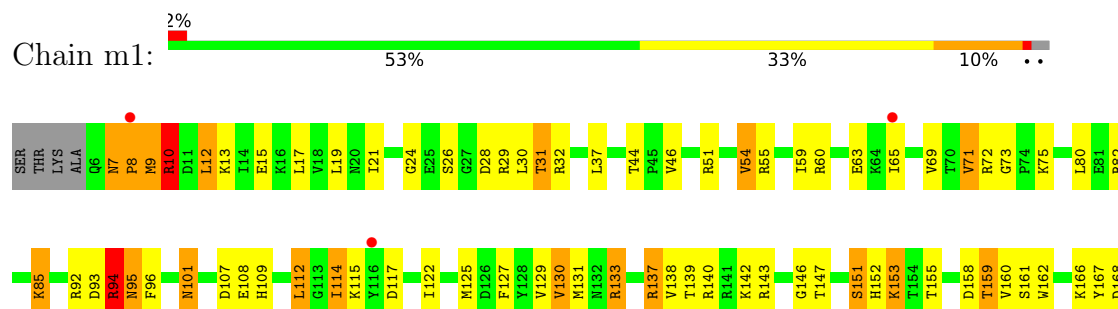
• Molecule 47: 60S ribosomal protein L10



• Molecule 48: 60S ribosomal protein L11-B



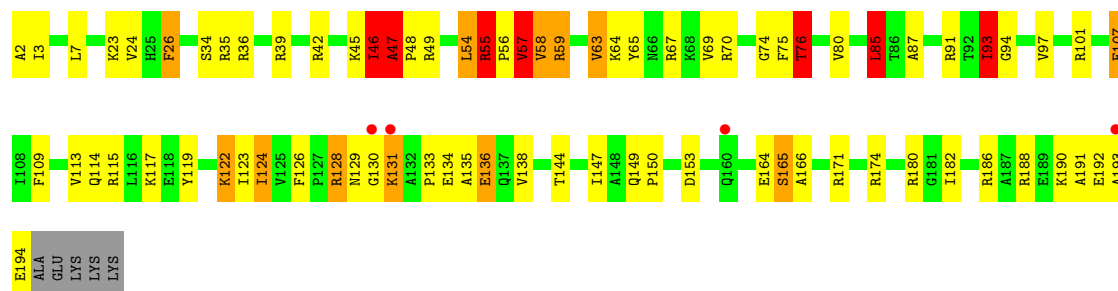
• Molecule 48: 60S ribosomal protein L11-B



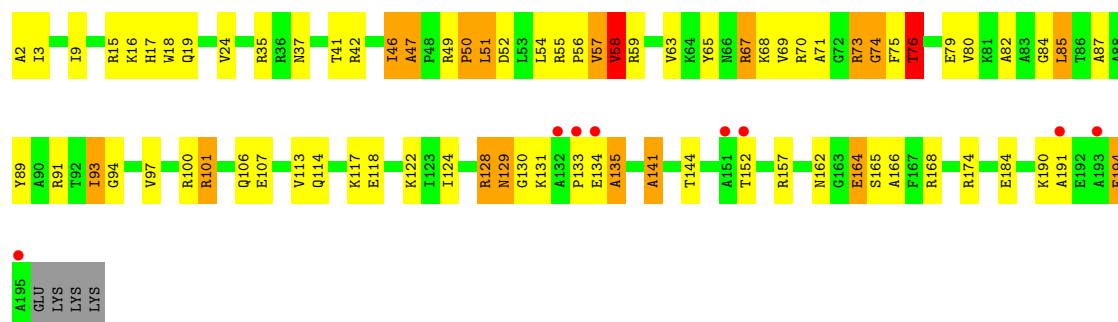




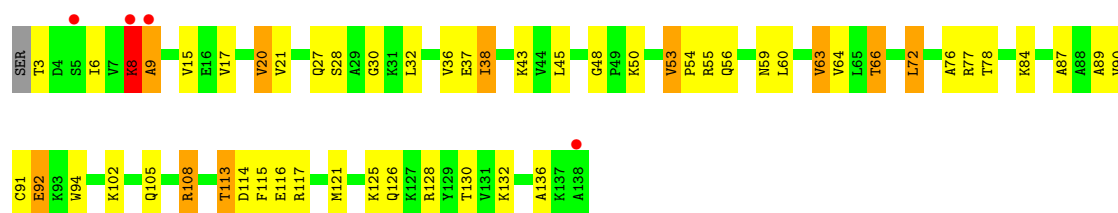
• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A



• Molecule 50: 60S ribosomal protein L14-A



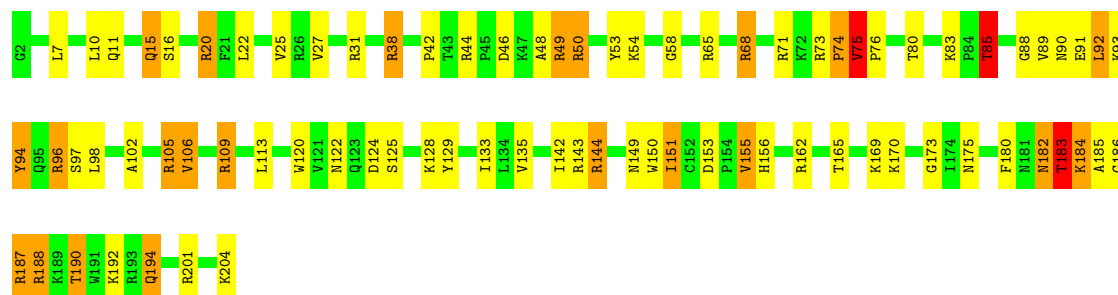
• Molecule 50: 60S ribosomal protein L14-A





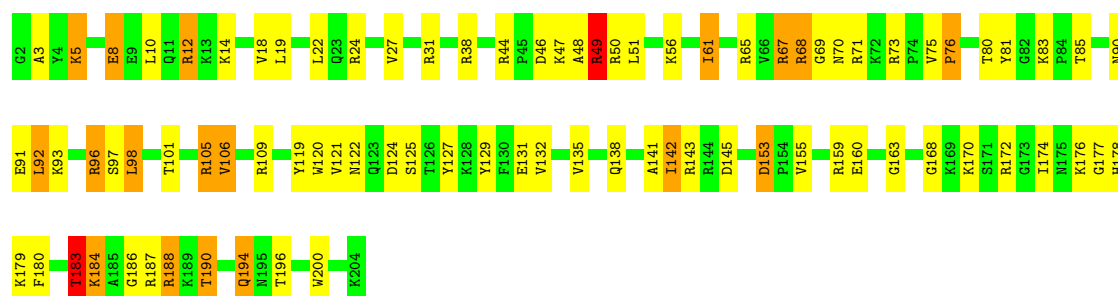
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 60% 28% 11% .



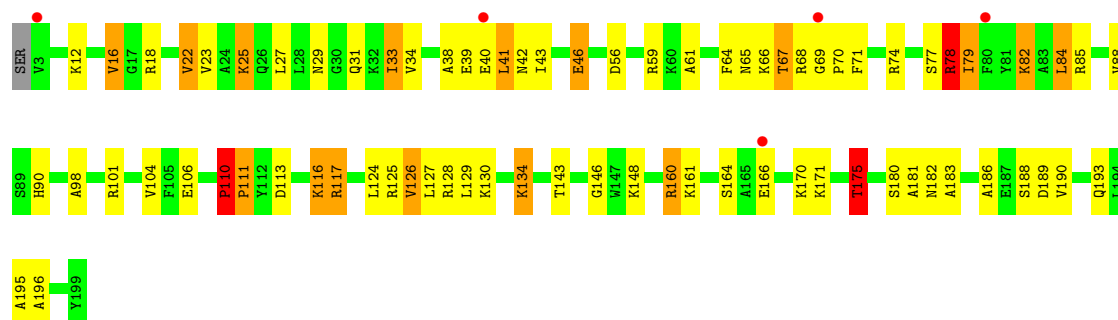
- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 58% 32% 9% .



- Molecule 52: 60S ribosomal protein L16-A

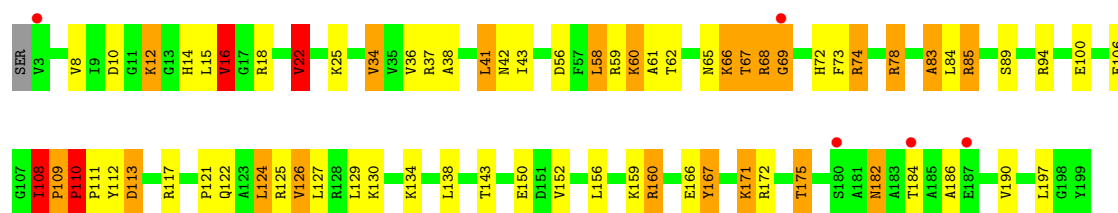
Chain M6: 3% 61% 29% 8% ..



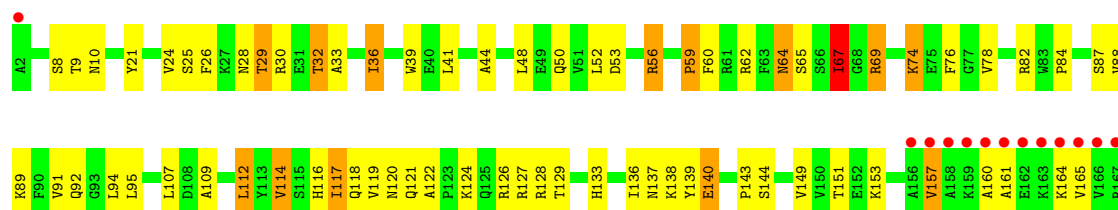
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 3% 64% 23% 11% ..

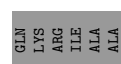
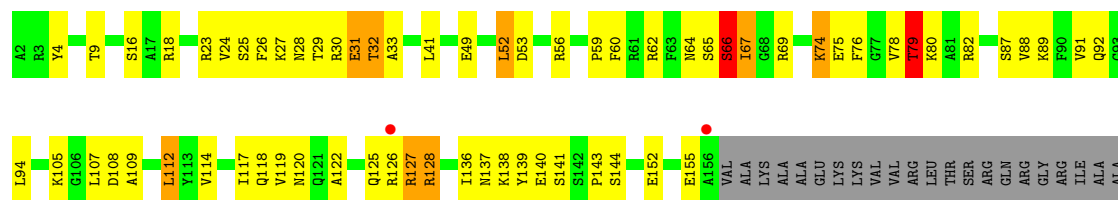




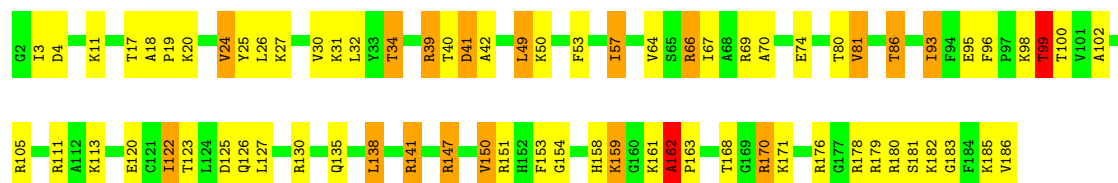
• Molecule 53: 60S ribosomal protein L17-A



• Molecule 53: 60S ribosomal protein L17-A

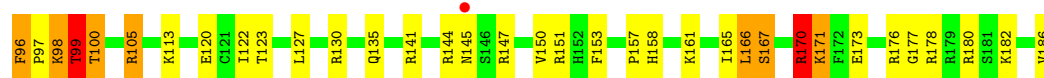
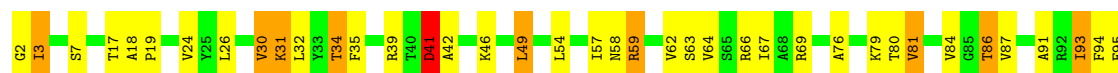


• Molecule 54: 60S ribosomal protein L18-A



• Molecule 54: 60S ribosomal protein L18-A

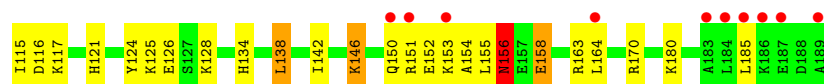




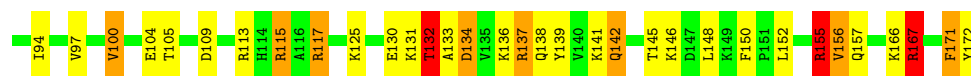
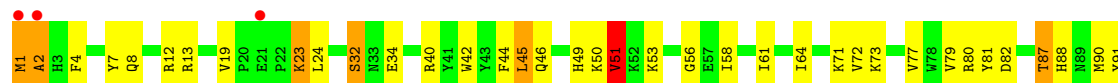
• Molecule 55: 60S ribosomal protein L19-A



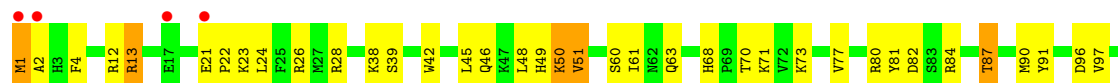
• Molecule 55: 60S ribosomal protein L19-A



• Molecule 56: 60S ribosomal protein L20-A



• Molecule 56: 60S ribosomal protein L20-A

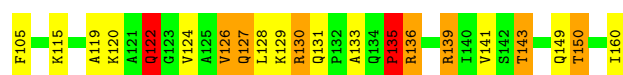
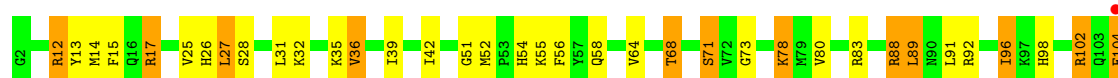




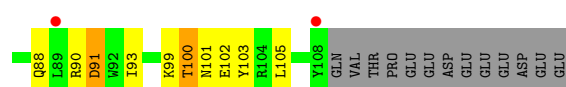
- Molecule 57: 60S ribosomal protein L21-A



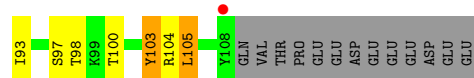
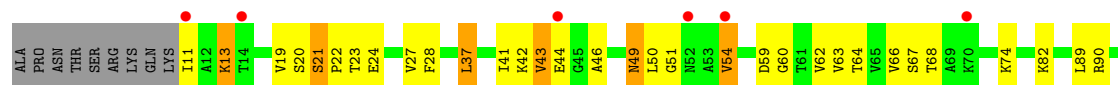
- Molecule 57: 60S ribosomal protein L21-A



- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



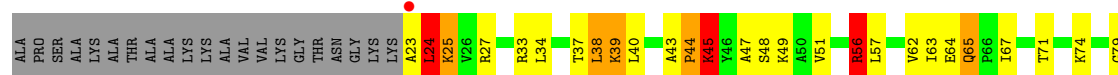
- Molecule 59: 60S ribosomal protein L23-A



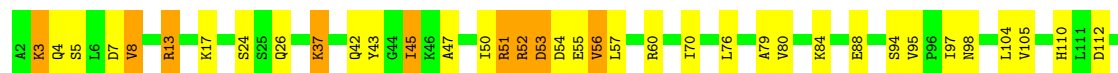




- Molecule 61: 60S ribosomal protein L25



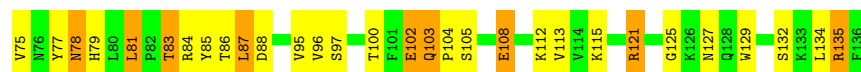
- Molecule 62: 60S ribosomal protein L26-A



- Molecule 62: 60S ribosomal protein L26-A



- Molecule 63: 60S ribosomal protein L27-A

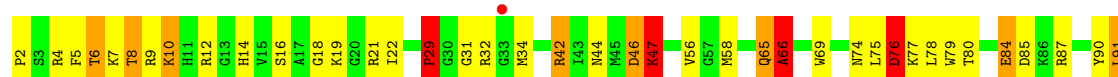


- Molecule 63: 60S ribosomal protein L27-A

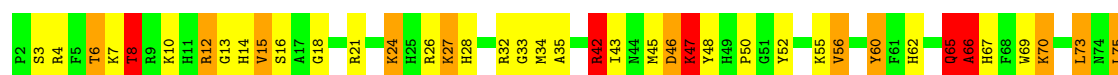




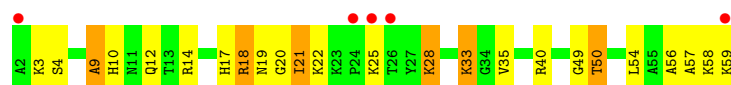
• Molecule 64: 60S ribosomal protein L28



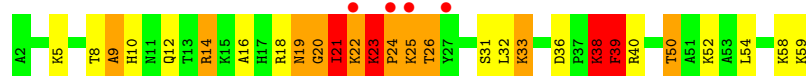
• Molecule 64: 60S ribosomal protein L28



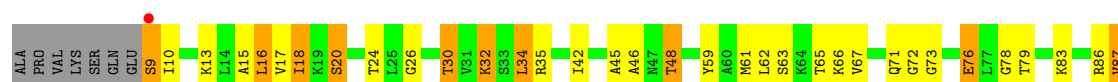
• Molecule 65: 60S ribosomal protein L29



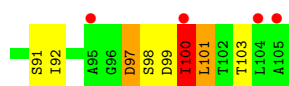
• Molecule 65: 60S ribosomal protein L29



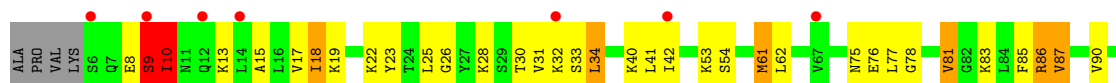
• Molecule 66: 60S ribosomal protein L30



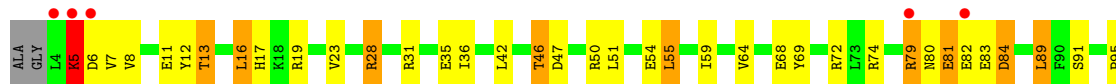




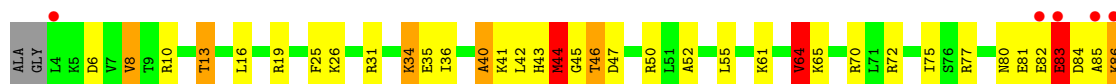
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A

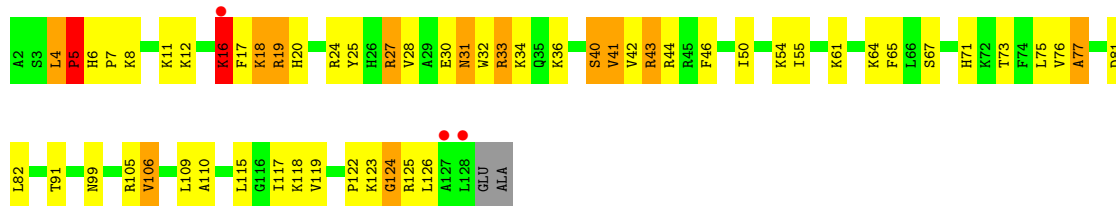


- Molecule 68: 60S ribosomal protein L32

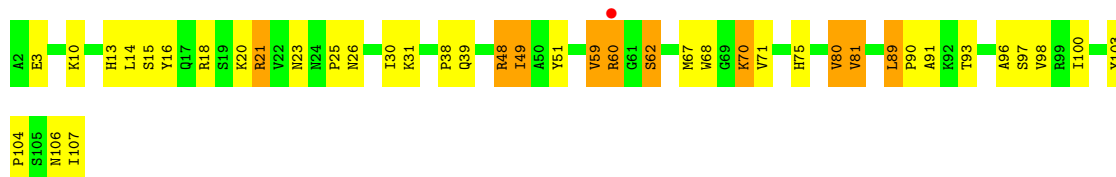


- Molecule 68: 60S ribosomal protein L32

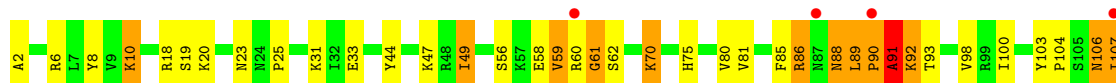




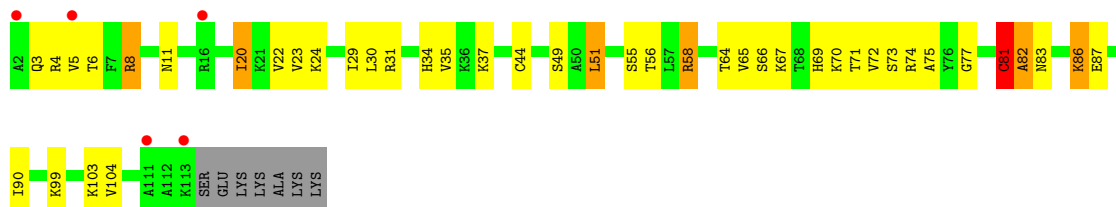
• Molecule 69: 60S ribosomal protein L33-A



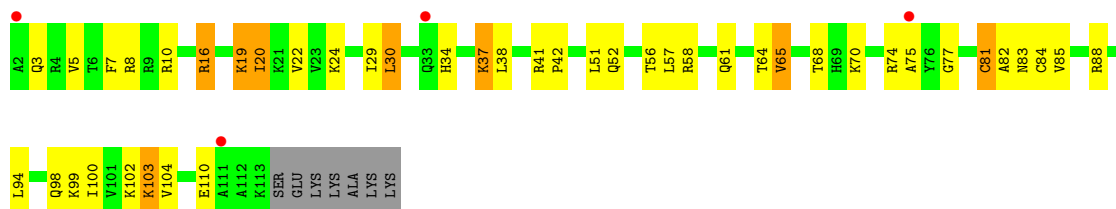
• Molecule 69: 60S ribosomal protein L33-A



• Molecule 70: 60S ribosomal protein L34-A

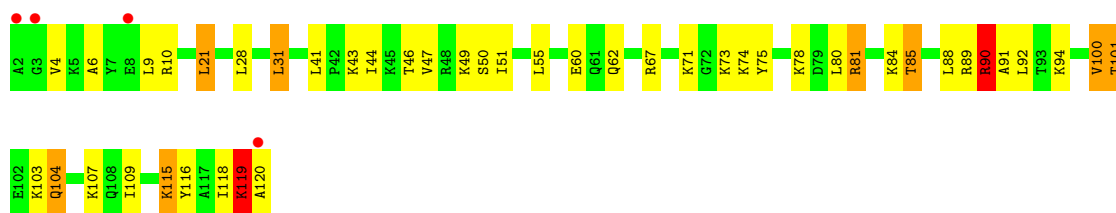


• Molecule 70: 60S ribosomal protein L34-A



• Molecule 71: 60S ribosomal protein L35-A

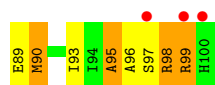
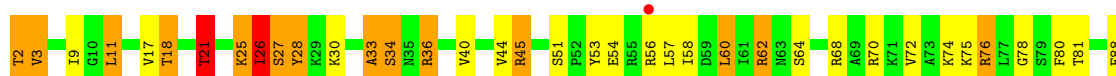




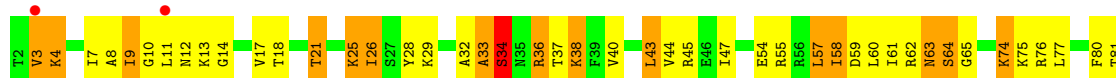
• Molecule 71: 60S ribosomal protein L35-A



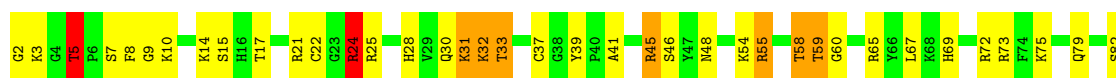
• Molecule 72: 60S ribosomal protein L36-A



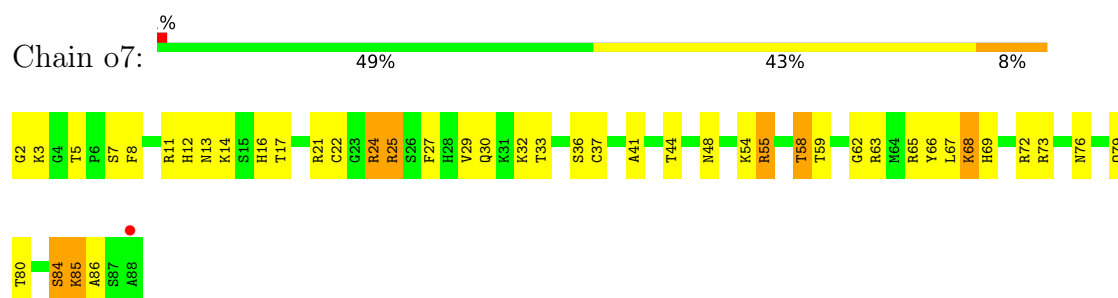
• Molecule 72: 60S ribosomal protein L36-A



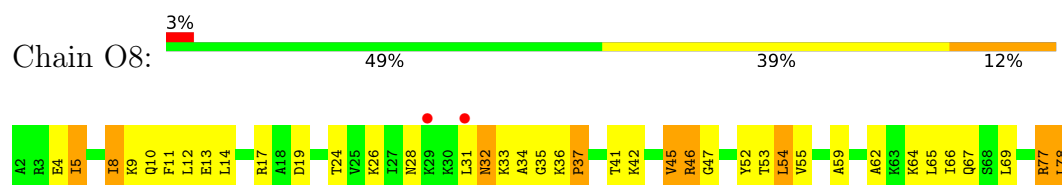
• Molecule 73: 60S ribosomal protein L37-A



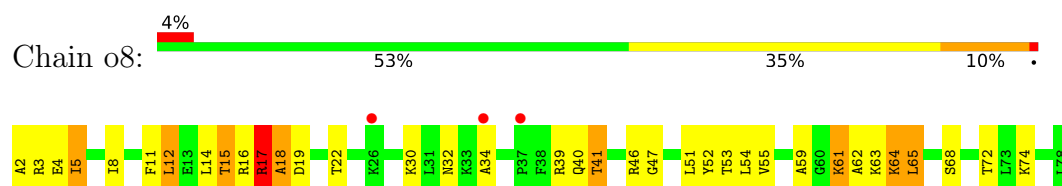
- Molecule 73: 60S ribosomal protein L37-A



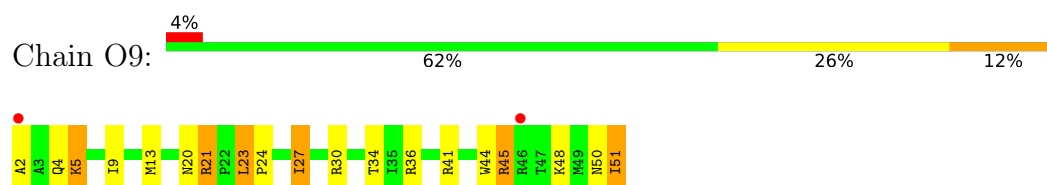
- Molecule 74: 60S ribosomal protein L38



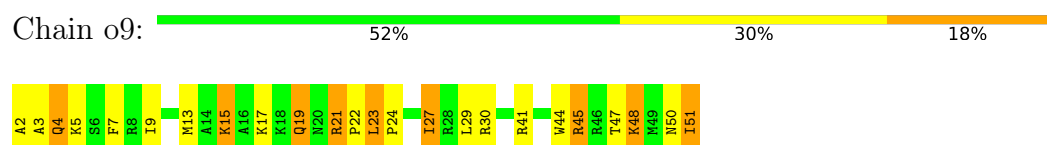
- Molecule 74: 60S ribosomal protein L38



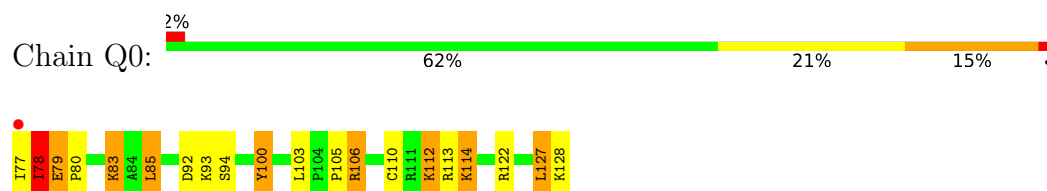
- Molecule 75: 60S ribosomal protein L39



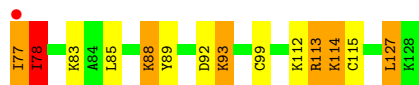
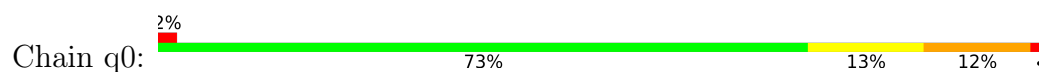
- Molecule 75: 60S ribosomal protein L39



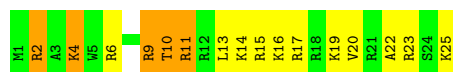
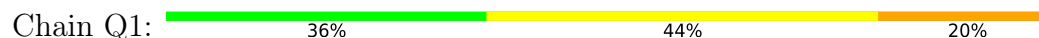
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



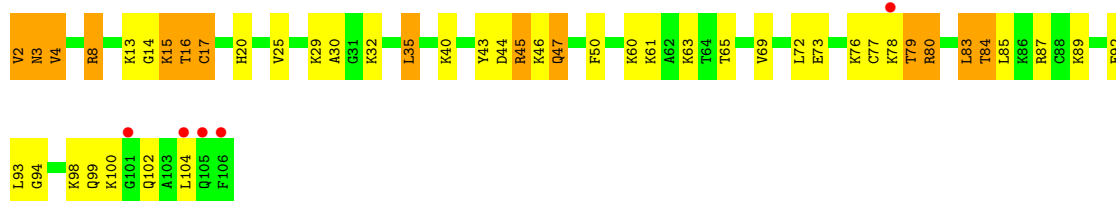
- Molecule 77: 60S ribosomal protein L41-A



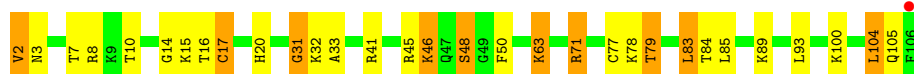
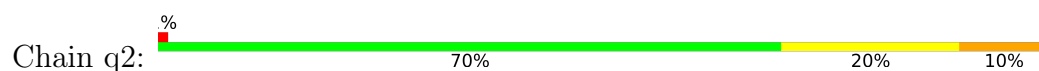
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A

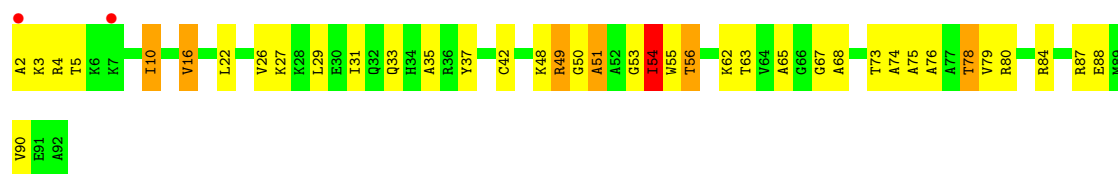


- Molecule 79: 60S ribosomal protein L43-A

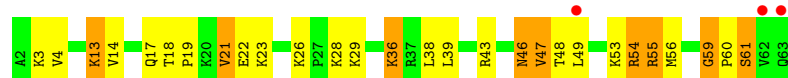


- Molecule 79: 60S ribosomal protein L43-A

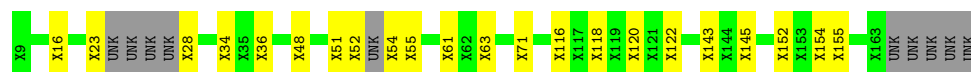
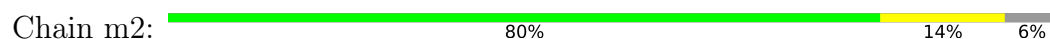




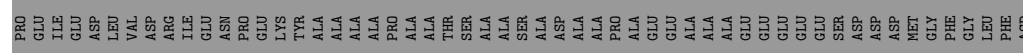
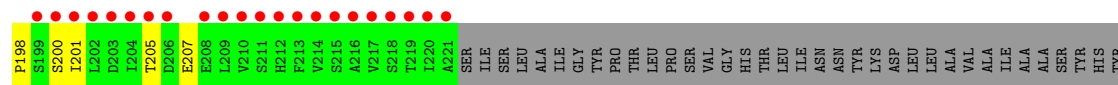
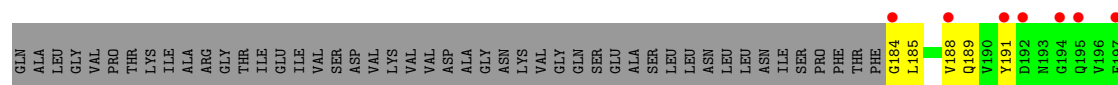
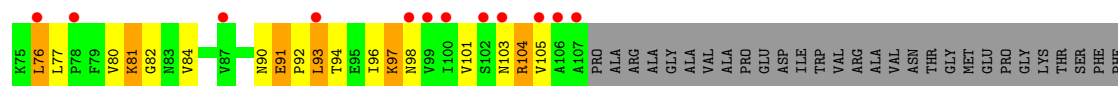
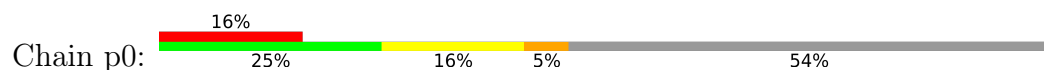
- Molecule 80: 40S ribosomal protein S30-A



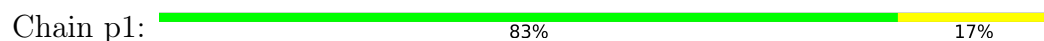
- Molecule 81: Unknown protein m2



- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: Unknown protein p1



- Molecule 84: Unknown protein p2



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 436.64Å 287.69Å 304.39Å<br>90.00° 98.98° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 300.66 – 2.80<br>300.66 – 2.80                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (300.66-2.80)<br>99.5 (300.66-2.80)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.25                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.36 (at 2.82Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1702)                            | Depositor        |
| R, $R_{free}$                                                           | 0.208 , 0.246<br>0.214 , 0.250                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 34000 reflections (1.88%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.227                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 59.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 411226                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, MG, ZN, 3H3

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   | 2     | 0.41         | 0/41698       | 0.62        | 7/64972 (0.0%) |
| 1   | 6     | 0.48         | 0/42765       | 0.67        | 8/66634 (0.0%) |
| 2   | S0    | 0.59         | 0/1617        | 1.07        | 10/2215 (0.5%) |
| 2   | s0    | 0.69         | 0/1623        | 1.15        | 7/2222 (0.3%)  |
| 3   | S1    | 0.50         | 0/1735        | 0.90        | 1/2335 (0.0%)  |
| 3   | s1    | 0.65         | 0/1748        | 1.04        | 7/2352 (0.3%)  |
| 4   | S2    | 0.66         | 0/1665        | 1.04        | 10/2263 (0.4%) |
| 4   | s2    | 0.80         | 0/1665        | 1.12        | 3/2263 (0.1%)  |
| 5   | S3    | 0.62         | 0/1759        | 1.00        | 3/2368 (0.1%)  |
| 5   | s3    | 0.60         | 0/1759        | 0.96        | 7/2368 (0.3%)  |
| 6   | S4    | 0.64         | 0/2109        | 1.04        | 6/2839 (0.2%)  |
| 6   | s4    | 0.71         | 0/2109        | 1.12        | 11/2839 (0.4%) |
| 7   | S5    | 0.56         | 0/1629        | 1.00        | 7/2202 (0.3%)  |
| 7   | s5    | 0.59         | 0/1629        | 1.02        | 9/2202 (0.4%)  |
| 8   | S6    | 0.60         | 0/1823        | 0.97        | 1/2439 (0.0%)  |
| 8   | s6    | 0.70         | 0/1779        | 1.01        | 6/2379 (0.3%)  |
| 9   | S7    | 0.57         | 0/1506        | 0.99        | 6/2028 (0.3%)  |
| 9   | s7    | 0.69         | 0/1516        | 1.11        | 5/2043 (0.2%)  |
| 10  | S8    | 0.72         | 0/1514        | 1.05        | 1/2021 (0.0%)  |
| 10  | s8    | 0.79         | 1/1514 (0.1%) | 1.05        | 0/2021         |
| 11  | S9    | 0.63         | 0/1519        | 1.02        | 4/2035 (0.2%)  |
| 11  | s9    | 0.71         | 0/1519        | 1.12        | 9/2035 (0.4%)  |
| 12  | C0    | 0.58         | 0/790         | 1.01        | 6/1069 (0.6%)  |
| 12  | c0    | 0.50         | 0/777         | 0.97        | 5/1049 (0.5%)  |
| 13  | C1    | 0.73         | 0/1240        | 1.05        | 4/1675 (0.2%)  |
| 13  | c1    | 0.83         | 0/1194        | 1.19        | 3/1610 (0.2%)  |
| 14  | C2    | 0.51         | 0/898         | 0.93        | 3/1220 (0.2%)  |
| 14  | c2    | 0.44         | 0/898         | 0.87        | 1/1220 (0.1%)  |
| 15  | C3    | 0.65         | 0/1215        | 1.02        | 6/1638 (0.4%)  |
| 15  | c3    | 0.77         | 0/1215        | 1.11        | 4/1638 (0.2%)  |
| 16  | C4    | 0.54         | 0/901         | 0.99        | 3/1217 (0.2%)  |
| 16  | c4    | 0.69         | 0/960         | 1.18        | 12/1290 (0.9%) |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | C5    | 0.64         | 0/998          | 1.00        | 4/1341 (0.3%)    |
| 17  | c5    | 0.64         | 0/1060         | 1.04        | 2/1426 (0.1%)    |
| 18  | C6    | 0.57         | 0/1125         | 1.05        | 4/1510 (0.3%)    |
| 18  | c6    | 0.65         | 0/1131         | 1.06        | 5/1518 (0.3%)    |
| 19  | C7    | 0.62         | 0/935          | 1.00        | 3/1254 (0.2%)    |
| 19  | c7    | 0.65         | 0/914          | 1.14        | 5/1224 (0.4%)    |
| 20  | C8    | 0.61         | 0/1211         | 1.02        | 4/1628 (0.2%)    |
| 20  | c8    | 0.65         | 1/1211 (0.1%)  | 1.02        | 1/1628 (0.1%)    |
| 21  | C9    | 0.62         | 0/1130         | 1.01        | 2/1517 (0.1%)    |
| 21  | c9    | 0.62         | 0/1130         | 1.00        | 1/1517 (0.1%)    |
| 22  | D0    | 0.61         | 0/865          | 0.98        | 1/1169 (0.1%)    |
| 22  | d0    | 0.63         | 0/892          | 1.08        | 4/1205 (0.3%)    |
| 23  | D1    | 0.59         | 0/693          | 1.00        | 3/935 (0.3%)     |
| 23  | d1    | 0.70         | 0/693          | 1.06        | 0/935            |
| 24  | D2    | 0.71         | 0/1038         | 1.10        | 3/1395 (0.2%)    |
| 24  | d2    | 0.86         | 0/1038         | 1.09        | 7/1395 (0.5%)    |
| 25  | D3    | 0.79         | 0/1139         | 1.21        | 11/1518 (0.7%)   |
| 25  | d3    | 0.87         | 0/1139         | 1.20        | 9/1518 (0.6%)    |
| 26  | D4    | 0.58         | 0/1087         | 0.95        | 2/1449 (0.1%)    |
| 26  | d4    | 0.65         | 0/1087         | 1.02        | 1/1449 (0.1%)    |
| 27  | D5    | 0.57         | 0/571          | 1.14        | 4/768 (0.5%)     |
| 27  | d5    | 0.60         | 0/566          | 0.98        | 0/761            |
| 28  | D6    | 0.63         | 0/782          | 1.04        | 5/1047 (0.5%)    |
| 28  | d6    | 0.73         | 0/782          | 1.03        | 0/1047           |
| 29  | D7    | 0.59         | 0/620          | 1.00        | 3/838 (0.4%)     |
| 29  | d7    | 0.65         | 0/620          | 1.15        | 4/838 (0.5%)     |
| 30  | D8    | 0.44         | 0/499          | 0.83        | 0/670            |
| 30  | d8    | 0.60         | 0/499          | 1.08        | 2/670 (0.3%)     |
| 31  | D9    | 0.68         | 0/452          | 1.01        | 3/600 (0.5%)     |
| 31  | d9    | 0.68         | 0/452          | 1.04        | 1/600 (0.2%)     |
| 32  | E0    | 0.60         | 0/483          | 0.97        | 0/643            |
| 33  | E1    | 0.65         | 0/577          | 1.16        | 4/770 (0.5%)     |
| 33  | e1    | 0.63         | 0/619          | 1.18        | 7/822 (0.9%)     |
| 34  | SR    | 1.57         | 2/2494 (0.1%)  | 2.00        | 10/3393 (0.3%)   |
| 34  | sR    | 0.52         | 0/2495         | 0.88        | 0/3395           |
| 35  | SM    | 0.74         | 0/1113         | 1.09        | 3/1502 (0.2%)    |
| 35  | sM    | 0.70         | 0/683          | 1.09        | 4/923 (0.4%)     |
| 36  | 1     | 0.63         | 0/75394        | 0.79        | 29/117545 (0.0%) |
| 36  | 5     | 0.65         | 2/75414 (0.0%) | 0.79        | 18/117575 (0.0%) |
| 37  | 3     | 0.52         | 0/2883         | 0.67        | 0/4491           |
| 37  | 7     | 0.61         | 0/2883         | 0.76        | 0/4491           |
| 38  | 4     | 0.62         | 0/3746         | 0.74        | 0/5832           |
| 38  | 8     | 0.55         | 0/3746         | 0.70        | 0/5832           |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 39  | L2    | 0.93         | 0/1948        | 1.21        | 8/2617 (0.3%)  |
| 39  | l2    | 1.04         | 3/1946 (0.2%) | 1.33        | 10/2614 (0.4%) |
| 40  | L3    | 0.95         | 3/3146 (0.1%) | 1.20        | 13/4228 (0.3%) |
| 40  | l3    | 1.04         | 3/3146 (0.1%) | 1.25        | 24/4228 (0.6%) |
| 41  | L4    | 1.05         | 2/2800 (0.1%) | 1.38        | 22/3790 (0.6%) |
| 41  | l4    | 0.98         | 1/2800 (0.0%) | 1.25        | 23/3790 (0.6%) |
| 42  | L5    | 0.70         | 0/2425        | 1.05        | 4/3271 (0.1%)  |
| 42  | l5    | 0.88         | 0/2408        | 1.15        | 7/3248 (0.2%)  |
| 43  | L6    | 0.95         | 1/1260 (0.1%) | 1.15        | 4/1694 (0.2%)  |
| 43  | l6    | 0.90         | 0/1269        | 1.17        | 5/1705 (0.3%)  |
| 44  | L7    | 1.03         | 1/1821 (0.1%) | 1.27        | 11/2451 (0.4%) |
| 44  | l7    | 1.03         | 0/1828        | 1.27        | 15/2461 (0.6%) |
| 45  | L8    | 0.71         | 0/1836        | 1.04        | 6/2481 (0.2%)  |
| 45  | l8    | 0.71         | 0/1795        | 1.02        | 5/2429 (0.2%)  |
| 46  | L9    | 0.81         | 0/1539        | 1.13        | 5/2073 (0.2%)  |
| 46  | l9    | 0.98         | 0/1539        | 1.20        | 5/2073 (0.2%)  |
| 47  | M0    | 0.92         | 0/1741        | 1.19        | 8/2335 (0.3%)  |
| 47  | m0    | 0.97         | 0/1758        | 1.16        | 8/2358 (0.3%)  |
| 48  | M1    | 0.68         | 0/1374        | 1.08        | 3/1842 (0.2%)  |
| 48  | m1    | 0.86         | 1/1374 (0.1%) | 1.21        | 7/1842 (0.4%)  |
| 49  | M3    | 0.98         | 3/1568 (0.2%) | 1.28        | 12/2106 (0.6%) |
| 49  | m3    | 0.97         | 1/1573 (0.1%) | 1.23        | 11/2113 (0.5%) |
| 50  | M4    | 1.00         | 1/1068 (0.1%) | 1.24        | 2/1438 (0.1%)  |
| 50  | m4    | 1.01         | 1/1074 (0.1%) | 1.22        | 4/1446 (0.3%)  |
| 51  | M5    | 0.96         | 2/1757 (0.1%) | 1.26        | 11/2354 (0.5%) |
| 51  | m5    | 0.88         | 0/1757        | 1.15        | 8/2354 (0.3%)  |
| 52  | M6    | 1.04         | 1/1585 (0.1%) | 1.22        | 7/2128 (0.3%)  |
| 52  | m6    | 1.20         | 1/1585 (0.1%) | 1.40        | 15/2128 (0.7%) |
| 53  | M7    | 0.99         | 0/1443        | 1.23        | 13/1944 (0.7%) |
| 53  | m7    | 1.11         | 1/1250 (0.1%) | 1.23        | 3/1683 (0.2%)  |
| 54  | M8    | 1.05         | 0/1465        | 1.37        | 8/1965 (0.4%)  |
| 54  | m8    | 0.96         | 0/1465        | 1.32        | 11/1965 (0.6%) |
| 55  | M9    | 0.73         | 0/1538        | 0.99        | 2/2050 (0.1%)  |
| 55  | m9    | 0.81         | 0/1538        | 1.03        | 2/2050 (0.1%)  |
| 56  | N0    | 1.01         | 0/1481        | 1.18        | 8/1990 (0.4%)  |
| 56  | n0    | 0.98         | 0/1481        | 1.23        | 7/1990 (0.4%)  |
| 57  | N1    | 0.95         | 1/1300 (0.1%) | 1.22        | 4/1743 (0.2%)  |
| 57  | n1    | 0.99         | 0/1300        | 1.17        | 4/1743 (0.2%)  |
| 58  | N2    | 0.52         | 0/812         | 0.93        | 1/1099 (0.1%)  |
| 58  | n2    | 0.61         | 0/794         | 1.01        | 4/1076 (0.4%)  |
| 59  | N3    | 0.95         | 0/1018        | 1.23        | 2/1369 (0.1%)  |
| 59  | n3    | 1.08         | 0/1018        | 1.30        | 5/1369 (0.4%)  |
| 60  | N4    | 0.74         | 0/712         | 1.30        | 2/958 (0.2%)   |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 60  | n4    | 0.82         | 0/1052           | 1.04        | 3/1398 (0.2%)     |
| 61  | N5    | 0.78         | 0/979            | 1.15        | 3/1321 (0.2%)     |
| 61  | n5    | 0.82         | 0/974            | 1.24        | 9/1314 (0.7%)     |
| 62  | N6    | 0.92         | 0/1004           | 1.12        | 3/1341 (0.2%)     |
| 62  | n6    | 0.81         | 0/1004           | 1.12        | 4/1341 (0.3%)     |
| 63  | N7    | 0.64         | 0/1118           | 1.07        | 2/1497 (0.1%)     |
| 63  | n7    | 0.61         | 0/1118           | 1.03        | 2/1497 (0.1%)     |
| 64  | N8    | 1.06         | 2/1204 (0.2%)    | 1.30        | 12/1612 (0.7%)    |
| 64  | n8    | 1.03         | 2/1204 (0.2%)    | 1.31        | 14/1612 (0.9%)    |
| 65  | N9    | 0.98         | 1/473 (0.2%)     | 1.06        | 2/629 (0.3%)      |
| 65  | n9    | 1.12         | 2/473 (0.4%)     | 1.35        | 9/629 (1.4%)      |
| 66  | O0    | 0.62         | 0/751            | 1.05        | 2/1008 (0.2%)     |
| 66  | o0    | 0.63         | 0/775            | 1.01        | 2/1040 (0.2%)     |
| 67  | O1    | 0.85         | 0/890            | 1.10        | 0/1196            |
| 67  | o1    | 1.02         | 1/897 (0.1%)     | 1.26        | 8/1205 (0.7%)     |
| 68  | O2    | 1.06         | 0/1041           | 1.19        | 2/1394 (0.1%)     |
| 68  | o2    | 1.07         | 2/1041 (0.2%)    | 1.27        | 9/1394 (0.6%)     |
| 69  | O3    | 1.05         | 0/868            | 1.19        | 3/1168 (0.3%)     |
| 69  | o3    | 1.16         | 4/868 (0.5%)     | 1.26        | 3/1168 (0.3%)     |
| 70  | O4    | 0.76         | 0/890            | 1.12        | 4/1189 (0.3%)     |
| 70  | o4    | 0.81         | 0/890            | 1.06        | 1/1189 (0.1%)     |
| 71  | O5    | 0.84         | 0/978            | 1.12        | 4/1301 (0.3%)     |
| 71  | o5    | 0.75         | 1/974 (0.1%)     | 1.01        | 4/1297 (0.3%)     |
| 72  | O6    | 0.89         | 0/778            | 1.20        | 4/1034 (0.4%)     |
| 72  | o6    | 0.73         | 0/777            | 1.06        | 3/1033 (0.3%)     |
| 73  | O7    | 1.05         | 0/696            | 1.28        | 6/923 (0.7%)      |
| 73  | o7    | 0.90         | 0/696            | 1.11        | 3/923 (0.3%)      |
| 74  | O8    | 0.60         | 0/618            | 0.97        | 0/826             |
| 74  | o8    | 0.63         | 0/614            | 1.07        | 1/822 (0.1%)      |
| 75  | O9    | 0.99         | 0/443            | 1.16        | 0/588             |
| 75  | o9    | 0.97         | 0/443            | 1.22        | 0/588             |
| 76  | Q0    | 0.88         | 0/423            | 1.16        | 3/562 (0.5%)      |
| 76  | q0    | 1.08         | 0/423            | 1.18        | 0/562             |
| 77  | Q1    | 0.82         | 0/234            | 1.05        | 0/300             |
| 77  | q1    | 1.03         | 0/234            | 1.24        | 1/300 (0.3%)      |
| 78  | Q2    | 1.00         | 1/860 (0.1%)     | 1.21        | 1/1136 (0.1%)     |
| 78  | q2    | 0.94         | 0/860            | 1.09        | 0/1136            |
| 79  | Q3    | 0.87         | 0/701            | 1.21        | 3/934 (0.3%)      |
| 79  | q3    | 0.92         | 1/701 (0.1%)     | 1.21        | 3/934 (0.3%)      |
| 80  | e0    | 0.69         | 0/499            | 1.22        | 2/665 (0.3%)      |
| 82  | p0    | 0.54         | 0/1092           | 0.96        | 0/1474            |
| All | All   | 0.70         | 50/430070 (0.0%) | 0.92        | 818/631356 (0.1%) |

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   | S0    | 0                   | 1                   |
| 7   | s5    | 0                   | 2                   |
| 9   | S7    | 0                   | 1                   |
| 10  | S8    | 0                   | 1                   |
| 16  | C4    | 0                   | 2                   |
| 17  | c5    | 0                   | 1                   |
| 19  | C7    | 0                   | 1                   |
| 22  | d0    | 0                   | 1                   |
| 25  | D3    | 0                   | 1                   |
| 25  | d3    | 0                   | 1                   |
| 26  | d4    | 0                   | 2                   |
| 27  | D5    | 0                   | 1                   |
| 28  | D6    | 0                   | 3                   |
| 31  | d9    | 0                   | 1                   |
| 33  | E1    | 0                   | 1                   |
| 34  | SR    | 0                   | 2                   |
| 39  | L2    | 0                   | 1                   |
| 39  | l2    | 0                   | 2                   |
| 40  | l3    | 0                   | 2                   |
| 41  | L4    | 0                   | 2                   |
| 41  | l4    | 0                   | 1                   |
| 42  | L5    | 0                   | 1                   |
| 42  | l5    | 0                   | 2                   |
| 43  | l6    | 0                   | 1                   |
| 44  | L7    | 0                   | 1                   |
| 44  | l7    | 0                   | 2                   |
| 51  | M5    | 0                   | 1                   |
| 52  | M6    | 0                   | 2                   |
| 52  | m6    | 0                   | 1                   |
| 53  | M7    | 0                   | 1                   |
| 53  | m7    | 0                   | 1                   |
| 57  | N1    | 0                   | 1                   |
| 59  | n3    | 0                   | 1                   |
| 62  | n6    | 0                   | 1                   |
| 63  | N7    | 0                   | 1                   |
| 63  | n7    | 0                   | 1                   |
| 64  | n8    | 0                   | 2                   |
| 65  | N9    | 0                   | 1                   |
| 65  | n9    | 0                   | 3                   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 67  | O1    | 0                   | 1                   |
| 67  | o1    | 0                   | 1                   |
| 72  | O6    | 0                   | 1                   |
| All | All   | 0                   | 57                  |

All (50) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 34  | SR    | 160  | GLU  | C-N   | -63.03 | 0.45        | 1.33     |
| 34  | SR    | 161  | LYS  | C-N   | -37.75 | 0.66        | 1.33     |
| 39  | l2    | 213  | GLY  | C-O   | 11.31  | 1.39        | 1.23     |
| 53  | m7    | 66   | SER  | C-O   | 9.96   | 1.36        | 1.24     |
| 78  | Q2    | 17   | CYS  | CB-SG | 8.56   | 2.09        | 1.81     |
| 48  | m1    | 9    | MET  | CA-C  | -7.29  | 1.48        | 1.52     |
| 64  | n8    | 15   | VAL  | C-O   | 7.09   | 1.32        | 1.24     |
| 52  | m6    | 66   | LYS  | CE-NZ | 7.01   | 1.70        | 1.49     |
| 67  | o1    | 40   | ALA  | C-O   | -6.38  | 1.16        | 1.24     |
| 39  | l2    | 48   | ILE  | CA-CB | 6.29   | 1.62        | 1.54     |
| 40  | l3    | 8    | ALA  | CA-CB | -6.18  | 1.44        | 1.54     |
| 69  | o3    | 106  | ASN  | CA-C  | -6.12  | 1.44        | 1.52     |
| 41  | L4    | 312  | VAL  | CA-CB | 6.11   | 1.62        | 1.54     |
| 64  | N8    | 47   | LYS  | N-CA  | 6.06   | 1.54        | 1.46     |
| 41  | l4    | 145  | ILE  | CA-CB | 6.06   | 1.61        | 1.54     |
| 64  | n8    | 66   | ALA  | CA-CB | 6.00   | 1.62        | 1.53     |
| 68  | o2    | 77   | ALA  | CA-CB | -5.92  | 1.44        | 1.53     |
| 39  | l2    | 214  | GLY  | C-O   | -5.85  | 1.19        | 1.24     |
| 69  | o3    | 91   | ALA  | N-CA  | 5.85   | 1.53        | 1.46     |
| 69  | o3    | 92   | LYS  | CE-NZ | 5.81   | 1.66        | 1.49     |
| 51  | M5    | 183  | THR  | CA-C  | -5.76  | 1.47        | 1.53     |
| 51  | M5    | 75   | VAL  | CA-CB | 5.74   | 1.61        | 1.54     |
| 49  | M3    | 57   | VAL  | CA-C  | -5.64  | 1.46        | 1.52     |
| 79  | q3    | 54   | ILE  | CA-CB | 5.61   | 1.60        | 1.54     |
| 40  | l3    | 258  | ALA  | CA-CB | -5.58  | 1.46        | 1.52     |
| 57  | N1    | 44   | ALA  | CA-CB | -5.55  | 1.45        | 1.53     |
| 52  | M6    | 195  | ALA  | CA-CB | -5.52  | 1.44        | 1.53     |
| 49  | M3    | 93   | ILE  | CA-CB | 5.42   | 1.60        | 1.54     |
| 41  | L4    | 316  | ASN  | CA-C  | -5.42  | 1.47        | 1.53     |
| 40  | l3    | 295  | ALA  | CA-CB | -5.41  | 1.45        | 1.53     |
| 71  | o5    | 44   | ILE  | CA-CB | 5.38   | 1.61        | 1.54     |
| 65  | n9    | 9    | ALA  | CA-CB | -5.31  | 1.44        | 1.53     |
| 36  | 5     | 1152 | G    | N9-C4 | -5.30  | 1.27        | 1.38     |
| 50  | M4    | 38   | ILE  | CA-CB | -5.28  | 1.47        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 40  | L3    | 256  | HIS  | CA-C   | -5.26 | 1.47        | 1.52     |
| 44  | L7    | 164  | SER  | N-CA   | 5.26  | 1.52        | 1.46     |
| 49  | m3    | 24   | VAL  | CA-CB  | -5.26 | 1.48        | 1.54     |
| 50  | m4    | 57   | ALA  | CA-CB  | -5.26 | 1.45        | 1.53     |
| 49  | M3    | 46   | ILE  | CA-CB  | 5.25  | 1.61        | 1.54     |
| 40  | L3    | 322  | ILE  | CA-CB  | -5.25 | 1.48        | 1.54     |
| 40  | L3    | 229  | VAL  | CA-C   | 5.22  | 1.59        | 1.52     |
| 65  | n9    | 21   | ILE  | CA-CB  | -5.21 | 1.47        | 1.54     |
| 20  | c8    | 14   | ILE  | CA-CB  | 5.19  | 1.61        | 1.54     |
| 69  | o3    | 90   | PRO  | C-O    | 5.17  | 1.31        | 1.24     |
| 43  | L6    | 86   | ALA  | CA-CB  | -5.09 | 1.46        | 1.53     |
| 65  | N9    | 9    | ALA  | CA-CB  | -5.08 | 1.44        | 1.53     |
| 68  | o2    | 43   | ARG  | CZ-NH2 | -5.07 | 1.26        | 1.33     |
| 64  | N8    | 66   | ALA  | CA-C   | -5.05 | 1.46        | 1.52     |
| 36  | 5     | 2874 | G    | P-O5'  | 5.02  | 1.67        | 1.59     |
| 10  | s8    | 183  | ILE  | CA-CB  | 5.00  | 1.60        | 1.54     |

All (818) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 34  | SR    | 161 | LYS  | O-C-N  | -58.54 | 44.74       | 122.59   |
| 34  | SR    | 160 | GLU  | CA-C-N | -56.30 | 14.02       | 121.54   |
| 34  | SR    | 160 | GLU  | C-N-CA | -56.30 | 14.02       | 121.54   |
| 34  | SR    | 160 | GLU  | O-C-N  | -24.85 | 89.54       | 122.59   |
| 60  | N4    | 80  | ARG  | CA-C-N | 17.64  | 141.89      | 119.84   |
| 60  | N4    | 80  | ARG  | C-N-CA | 17.64  | 141.89      | 119.84   |
| 54  | M8    | 18  | ALA  | CA-C-N | -13.66 | 106.09      | 120.85   |
| 54  | M8    | 18  | ALA  | C-N-CA | -13.66 | 106.09      | 120.85   |
| 59  | n3    | 42  | SER  | N-CA-C | 11.80  | 124.93      | 110.41   |
| 25  | d3    | 130 | VAL  | N-CA-C | 11.16  | 120.94      | 111.90   |
| 49  | m3    | 47  | ALA  | CA-C-N | -11.05 | 107.51      | 120.89   |
| 49  | m3    | 47  | ALA  | C-N-CA | -11.05 | 107.51      | 120.89   |
| 9   | s7    | 185 | ILE  | CA-C-N | -11.05 | 106.03      | 119.84   |
| 9   | s7    | 185 | ILE  | C-N-CA | -11.05 | 106.03      | 119.84   |
| 15  | c3    | 136 | PRO  | CA-C-N | 10.96  | 133.55      | 119.84   |
| 15  | c3    | 136 | PRO  | C-N-CA | 10.96  | 133.55      | 119.84   |
| 39  | l2    | 214 | GLY  | N-CA-C | 10.89  | 125.85      | 112.79   |
| 39  | l2    | 55  | GLY  | N-CA-C | -10.56 | 100.72      | 112.33   |
| 54  | m8    | 18  | ALA  | CA-C-N | -10.30 | 109.22      | 120.14   |
| 54  | m8    | 18  | ALA  | C-N-CA | -10.30 | 109.22      | 120.14   |
| 18  | c6    | 40  | GLU  | CA-C-N | -10.20 | 109.83      | 119.82   |
| 18  | c6    | 40  | GLU  | C-N-CA | -10.20 | 109.83      | 119.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 61  | n5    | 43   | ALA  | CA-C-N      | 10.17  | 132.55      | 119.84   |
| 61  | n5    | 43   | ALA  | C-N-CA      | 10.17  | 132.55      | 119.84   |
| 9   | s7    | 131  | PHE  | CA-C-N      | -10.04 | 110.09      | 120.03   |
| 9   | s7    | 131  | PHE  | C-N-CA      | -10.04 | 110.09      | 120.03   |
| 52  | m6    | 109  | PRO  | CA-C-N      | 9.84   | 130.51      | 120.38   |
| 52  | m6    | 109  | PRO  | C-N-CA      | 9.84   | 130.51      | 120.38   |
| 41  | L4    | 3    | ARG  | CA-C-N      | 9.73   | 132.00      | 119.84   |
| 41  | L4    | 3    | ARG  | C-N-CA      | 9.73   | 132.00      | 119.84   |
| 39  | l2    | 216  | HIS  | N-CA-C      | -9.72  | 94.16       | 109.23   |
| 34  | SR    | 161  | LYS  | CA-C-N      | 9.60   | 139.69      | 122.31   |
| 34  | SR    | 161  | LYS  | C-N-CA      | 9.60   | 139.69      | 122.31   |
| 41  | L4    | 221  | ASN  | CA-C-N      | -9.56  | 115.71      | 122.59   |
| 41  | L4    | 221  | ASN  | C-N-CA      | -9.56  | 115.71      | 122.59   |
| 19  | c7    | 117  | LEU  | CA-C-N      | 9.44   | 130.95      | 120.66   |
| 19  | c7    | 117  | LEU  | C-N-CA      | 9.44   | 130.95      | 120.66   |
| 25  | D3    | 130  | VAL  | N-CA-C      | 9.44   | 119.07      | 111.62   |
| 52  | m6    | 108  | ILE  | CA-C-N      | 9.13   | 129.79      | 120.38   |
| 52  | m6    | 108  | ILE  | C-N-CA      | 9.13   | 129.79      | 120.38   |
| 47  | M0    | 169  | LYS  | N-CA-C      | -8.98  | 102.47      | 113.97   |
| 7   | S5    | 29   | ILE  | CA-C-N      | 8.98   | 129.06      | 119.90   |
| 7   | S5    | 29   | ILE  | C-N-CA      | 8.98   | 129.06      | 119.90   |
| 27  | D5    | 54   | VAL  | CA-C-N      | -8.95  | 111.62      | 120.21   |
| 27  | D5    | 54   | VAL  | C-N-CA      | -8.95  | 111.62      | 120.21   |
| 39  | l2    | 232  | GLY  | N-CA-C      | -8.81  | 103.26      | 114.37   |
| 42  | l5    | 271  | LYS  | N-CA-C      | -8.80  | 102.62      | 112.57   |
| 52  | m6    | 69   | GLY  | N-CA-C      | -8.74  | 94.51       | 112.34   |
| 52  | m6    | 110  | PRO  | CA-C-N      | -8.72  | 109.35      | 119.47   |
| 52  | m6    | 110  | PRO  | C-N-CA      | -8.72  | 109.35      | 119.47   |
| 20  | C8    | 145  | ARG  | CB-CA-C     | -8.67  | 106.57      | 116.54   |
| 18  | C6    | 40   | GLU  | C-N-CD      | -8.49  | 101.91      | 120.60   |
| 16  | c4    | 91   | THR  | N-CA-C      | 8.42   | 121.39      | 111.71   |
| 41  | L4    | 204  | GLY  | CA-C-N      | -8.40  | 111.72      | 120.03   |
| 41  | L4    | 204  | GLY  | C-N-CA      | -8.40  | 111.72      | 120.03   |
| 36  | 5     | 1307 | G    | C2'-C3'-O3' | 8.35   | 122.03      | 109.50   |
| 48  | m1    | 9    | MET  | O-C-N       | 8.32   | 128.19      | 120.71   |
| 54  | M8    | 162  | ALA  | CA-C-N      | 8.19   | 128.26      | 119.90   |
| 54  | M8    | 162  | ALA  | C-N-CA      | 8.19   | 128.26      | 119.90   |
| 80  | e0    | 59   | GLY  | CA-C-N      | 8.19   | 130.07      | 119.84   |
| 80  | e0    | 59   | GLY  | C-N-CA      | 8.19   | 130.07      | 119.84   |
| 35  | SM    | 38   | PRO  | CA-C-N      | 8.13   | 128.76      | 120.38   |
| 35  | SM    | 38   | PRO  | C-N-CA      | 8.13   | 128.76      | 120.38   |
| 20  | C8    | 140  | THR  | N-CA-C      | 8.12   | 120.21      | 111.36   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 49  | M3    | 7   | LEU  | CA-C-N      | -8.11 | 111.66      | 119.85   |
| 49  | M3    | 7   | LEU  | C-N-CA      | -8.11 | 111.66      | 119.85   |
| 64  | N8    | 14  | HIS  | CA-C-N      | -8.10 | 108.23      | 121.34   |
| 64  | N8    | 14  | HIS  | C-N-CA      | -8.10 | 108.23      | 121.34   |
| 29  | d7    | 37  | CYS  | CA-C-N      | 8.09  | 129.95      | 119.84   |
| 29  | d7    | 37  | CYS  | C-N-CA      | 8.09  | 129.95      | 119.84   |
| 45  | L8    | 158 | ASP  | CA-C-N      | -8.05 | 109.78      | 119.84   |
| 45  | L8    | 158 | ASP  | C-N-CA      | -8.05 | 109.78      | 119.84   |
| 2   | s0    | 3   | LEU  | CA-C-N      | 8.04  | 129.89      | 119.84   |
| 2   | s0    | 3   | LEU  | C-N-CA      | 8.04  | 129.89      | 119.84   |
| 51  | M5    | 185 | ALA  | N-CA-C      | -8.02 | 103.40      | 113.02   |
| 73  | O7    | 24  | ARG  | N-CA-C      | 8.01  | 122.87      | 113.18   |
| 6   | s4    | 30  | ARG  | CA-C-N      | 8.00  | 128.49      | 119.93   |
| 6   | s4    | 30  | ARG  | C-N-CA      | 8.00  | 128.49      | 119.93   |
| 18  | C6    | 40  | GLU  | CA-C-N      | 7.95  | 146.09      | 127.00   |
| 18  | C6    | 40  | GLU  | C-N-CA      | 7.95  | 146.09      | 127.00   |
| 52  | M6    | 110 | PRO  | CA-C-N      | 7.93  | 129.75      | 119.84   |
| 52  | M6    | 110 | PRO  | C-N-CA      | 7.93  | 129.75      | 119.84   |
| 25  | d3    | 129 | GLY  | CA-C-N      | -7.91 | 114.98      | 122.66   |
| 25  | d3    | 129 | GLY  | C-N-CA      | -7.91 | 114.98      | 122.66   |
| 12  | C0    | 88  | PRO  | N-CA-CB     | 7.88  | 111.53      | 103.25   |
| 36  | 1     | 65  | A    | C2'-C3'-O3' | 7.82  | 121.23      | 109.50   |
| 22  | d0    | 70  | THR  | CA-C-N      | -7.78 | 112.69      | 120.31   |
| 22  | d0    | 70  | THR  | C-N-CA      | -7.78 | 112.69      | 120.31   |
| 3   | S1    | 178 | GLY  | N-CA-C      | -7.75 | 101.96      | 112.57   |
| 41  | L4    | 222 | VAL  | CA-C-N      | 7.74  | 129.52      | 119.84   |
| 41  | L4    | 222 | VAL  | C-N-CA      | 7.74  | 129.52      | 119.84   |
| 50  | m4    | 72  | LEU  | CA-C-N      | -7.73 | 112.04      | 119.85   |
| 50  | m4    | 72  | LEU  | C-N-CA      | -7.73 | 112.04      | 119.85   |
| 43  | l6    | 94  | GLU  | N-CA-C      | 7.71  | 119.68      | 111.28   |
| 69  | o3    | 89  | LEU  | CA-C-N      | 7.67  | 127.38      | 119.56   |
| 69  | o3    | 89  | LEU  | C-N-CA      | 7.67  | 127.38      | 119.56   |
| 52  | m6    | 22  | VAL  | N-CA-C      | -7.62 | 103.03      | 110.72   |
| 61  | n5    | 65  | GLN  | CA-C-N      | -7.59 | 112.52      | 120.03   |
| 61  | n5    | 65  | GLN  | C-N-CA      | -7.59 | 112.52      | 120.03   |
| 13  | c1    | 128 | CYS  | N-CA-C      | 7.58  | 121.96      | 112.03   |
| 6   | S4    | 105 | VAL  | N-CA-C      | -7.55 | 105.95      | 113.20   |
| 35  | SM    | 167 | PRO  | N-CA-CB     | 7.55  | 111.18      | 103.25   |
| 54  | M8    | 99  | THR  | N-CA-C      | 7.55  | 126.89      | 110.80   |
| 42  | l5    | 37  | VAL  | N-CA-C      | 7.53  | 118.32      | 110.72   |
| 69  | O3    | 89  | LEU  | CA-C-N      | 7.50  | 127.21      | 119.56   |
| 69  | O3    | 89  | LEU  | C-N-CA      | 7.50  | 127.21      | 119.56   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | s0    | 167  | LYS  | CB-CA-C     | -7.50 | 107.92      | 116.54   |
| 1   | 2     | 1761 | U    | C2'-C3'-O3' | 7.50  | 120.74      | 109.50   |
| 68  | o2    | 16   | LYS  | N-CA-C      | 7.50  | 120.10      | 111.11   |
| 78  | Q2    | 35   | LEU  | N-CA-C      | -7.48 | 101.21      | 110.41   |
| 36  | 5     | 282  | G    | C2'-C3'-O3' | 7.45  | 124.87      | 113.70   |
| 41  | l4    | 198  | ARG  | N-CA-C      | 7.44  | 119.39      | 111.28   |
| 36  | 1     | 1329 | U    | N1-C1'-C2'  | -7.42 | 102.87      | 114.00   |
| 44  | l7    | 92   | ILE  | N-CA-C      | 7.41  | 120.16      | 112.83   |
| 64  | N8    | 66   | ALA  | N-CA-C      | -7.39 | 95.06       | 110.80   |
| 25  | D3    | 87   | VAL  | CA-C-N      | 7.38  | 127.80      | 119.83   |
| 25  | D3    | 87   | VAL  | C-N-CA      | 7.38  | 127.80      | 119.83   |
| 41  | L4    | 139  | GLY  | N-CA-C      | -7.37 | 98.81       | 112.37   |
| 59  | n3    | 65   | GLY  | CA-C-O      | -7.37 | 116.11      | 122.16   |
| 2   | S0    | 3    | LEU  | CA-C-N      | 7.36  | 129.04      | 119.84   |
| 2   | S0    | 3    | LEU  | C-N-CA      | 7.36  | 129.04      | 119.84   |
| 51  | m5    | 153  | ASP  | CA-C-N      | -7.34 | 112.23      | 119.87   |
| 51  | m5    | 153  | ASP  | C-N-CA      | -7.34 | 112.23      | 119.87   |
| 65  | n9    | 38   | LYS  | N-CA-C      | -7.34 | 98.95       | 109.96   |
| 24  | D2    | 55   | ASP  | N-CA-C      | -7.32 | 100.87      | 110.53   |
| 2   | s0    | 108  | THR  | N-CA-C      | -7.31 | 100.68      | 110.55   |
| 13  | C1    | 131  | ILE  | N-CA-C      | -7.31 | 104.87      | 113.42   |
| 44  | L7    | 98   | LYS  | CA-C-N      | -7.31 | 111.44      | 119.19   |
| 44  | L7    | 98   | LYS  | C-N-CA      | -7.31 | 111.44      | 119.19   |
| 40  | l3    | 129  | ALA  | CA-C-N      | -7.31 | 110.88      | 122.79   |
| 40  | l3    | 129  | ALA  | C-N-CA      | -7.31 | 110.88      | 122.79   |
| 52  | M6    | 69   | GLY  | N-CA-C      | -7.28 | 97.50       | 112.34   |
| 49  | M3    | 75   | PHE  | N-CA-C      | 7.26  | 122.24      | 113.23   |
| 48  | M1    | 23   | VAL  | CB-CA-C     | -7.24 | 105.11      | 113.22   |
| 51  | M5    | 192  | LYS  | N-CA-C      | -7.24 | 103.47      | 111.36   |
| 12  | c0    | 97   | PRO  | N-CA-CB     | 7.23  | 110.84      | 103.25   |
| 41  | L4    | 57   | GLY  | N-CA-C      | -7.22 | 106.10      | 114.69   |
| 16  | c4    | 123  | SER  | N-CA-C      | -7.21 | 102.91      | 112.72   |
| 64  | n8    | 46   | ASP  | N-CA-C      | -7.19 | 100.36      | 110.50   |
| 41  | L4    | 22   | LEU  | CA-C-N      | 7.17  | 128.81      | 119.84   |
| 41  | L4    | 22   | LEU  | C-N-CA      | 7.17  | 128.81      | 119.84   |
| 34  | SR    | 286  | GLU  | CA-C-N      | 7.16  | 126.92      | 119.76   |
| 34  | SR    | 286  | GLU  | C-N-CA      | 7.16  | 126.92      | 119.76   |
| 15  | C3    | 22   | ALA  | CA-C-N      | 7.16  | 144.18      | 127.00   |
| 15  | C3    | 22   | ALA  | C-N-CA      | 7.16  | 144.18      | 127.00   |
| 41  | L4    | 316  | ASN  | CA-C-N      | -7.15 | 110.90      | 119.84   |
| 41  | L4    | 316  | ASN  | C-N-CA      | -7.15 | 110.90      | 119.84   |
| 11  | s9    | 4    | ALA  | CA-C-N      | 7.13  | 128.76      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | s9    | 4    | ALA  | C-N-CA      | 7.13  | 128.76      | 119.84   |
| 40  | l3    | 184  | ASN  | CA-C-N      | -7.13 | 111.79      | 121.06   |
| 40  | l3    | 184  | ASN  | C-N-CA      | -7.13 | 111.79      | 121.06   |
| 7   | s5    | 27   | THR  | CA-C-N      | 7.13  | 128.75      | 119.84   |
| 7   | s5    | 27   | THR  | C-N-CA      | 7.13  | 128.75      | 119.84   |
| 49  | M3    | 47   | ALA  | CA-C-N      | -7.13 | 112.27      | 120.89   |
| 49  | M3    | 47   | ALA  | C-N-CA      | -7.13 | 112.27      | 120.89   |
| 51  | m5    | 177  | GLY  | N-CA-C      | 7.13  | 119.83      | 111.63   |
| 51  | m5    | 67   | ARG  | N-CA-C      | 7.09  | 121.76      | 113.18   |
| 35  | sM    | 167  | PRO  | N-CA-CB     | 7.08  | 110.69      | 103.25   |
| 16  | c4    | 119  | THR  | CA-C-N      | 7.07  | 127.50      | 119.93   |
| 16  | c4    | 119  | THR  | C-N-CA      | 7.07  | 127.50      | 119.93   |
| 15  | C3    | 22   | ALA  | C-N-CD      | -7.06 | 105.06      | 120.60   |
| 2   | S0    | 103  | THR  | CA-C-N      | 7.04  | 126.80      | 119.76   |
| 2   | S0    | 103  | THR  | C-N-CA      | 7.04  | 126.80      | 119.76   |
| 40  | L3    | 25   | ILE  | CB-CA-C     | -7.03 | 101.78      | 112.05   |
| 40  | l3    | 8    | ALA  | CA-C-N      | -7.03 | 112.75      | 119.85   |
| 40  | l3    | 8    | ALA  | C-N-CA      | -7.03 | 112.75      | 119.85   |
| 24  | D2    | 76   | SER  | CA-C-N      | -7.02 | 112.41      | 119.99   |
| 24  | D2    | 76   | SER  | C-N-CA      | -7.02 | 112.41      | 119.99   |
| 29  | d7    | 27   | GLY  | CA-C-N      | 7.02  | 126.99      | 119.76   |
| 29  | d7    | 27   | GLY  | C-N-CA      | 7.02  | 126.99      | 119.76   |
| 6   | s4    | 149  | TYR  | CA-C-N      | -6.99 | 113.47      | 120.31   |
| 6   | s4    | 149  | TYR  | C-N-CA      | -6.99 | 113.47      | 120.31   |
| 28  | D6    | 11   | ASN  | N-CA-C      | 6.98  | 120.87      | 111.24   |
| 41  | L4    | 327  | LEU  | N-CA-C      | -6.97 | 101.84      | 110.41   |
| 10  | S8    | 148  | ALA  | N-CA-C      | -6.97 | 103.16      | 113.40   |
| 63  | n7    | 27   | LYS  | CA-C-N      | 6.96  | 128.55      | 119.84   |
| 63  | n7    | 27   | LYS  | C-N-CA      | 6.96  | 128.55      | 119.84   |
| 5   | s3    | 219  | ALA  | CA-C-N      | 6.96  | 128.54      | 119.84   |
| 5   | s3    | 219  | ALA  | C-N-CA      | 6.96  | 128.54      | 119.84   |
| 36  | 1     | 406  | G    | O4'-C1'-N9  | 6.96  | 118.64      | 108.20   |
| 72  | O6    | 27   | SER  | N-CA-C      | -6.96 | 100.01      | 110.24   |
| 54  | M8    | 170  | ARG  | N-CA-C      | -6.95 | 100.89      | 110.35   |
| 54  | M8    | 18   | ALA  | N-CA-C      | -6.93 | 101.91      | 108.07   |
| 73  | O7    | 5    | THR  | CA-C-N      | -6.92 | 111.67      | 119.28   |
| 73  | O7    | 5    | THR  | C-N-CA      | -6.92 | 111.67      | 119.28   |
| 25  | D3    | 45   | GLY  | N-CA-C      | -6.91 | 105.21      | 114.95   |
| 6   | S4    | 76   | VAL  | N-CA-C      | 6.91  | 116.91      | 110.42   |
| 53  | M7    | 64   | ASN  | CA-C-N      | -6.89 | 111.65      | 121.50   |
| 53  | M7    | 64   | ASN  | C-N-CA      | -6.89 | 111.65      | 121.50   |
| 36  | 1     | 1307 | G    | C2'-C3'-O3' | 6.88  | 119.83      | 109.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 2     | 1339 | C    | C2'-C3'-O3' | 6.87  | 119.81      | 109.50   |
| 9   | S7    | 62   | VAL  | CA-C-N      | 6.81  | 128.35      | 119.84   |
| 9   | S7    | 62   | VAL  | C-N-CA      | 6.81  | 128.35      | 119.84   |
| 36  | 1     | 1329 | U    | C4'-C3'-O3' | 6.79  | 119.58      | 109.40   |
| 48  | m1    | 9    | MET  | N-CA-C      | -6.79 | 97.33       | 108.12   |
| 12  | c0    | 83   | PRO  | N-CA-CB     | 6.78  | 110.37      | 103.25   |
| 39  | l2    | 238  | ILE  | CA-C-N      | -6.78 | 108.59      | 121.54   |
| 39  | l2    | 238  | ILE  | C-N-CA      | -6.78 | 108.59      | 121.54   |
| 28  | D6    | 64   | LEU  | CA-C-N      | 6.77  | 128.30      | 119.84   |
| 28  | D6    | 64   | LEU  | C-N-CA      | 6.77  | 128.30      | 119.84   |
| 47  | m0    | 62   | SER  | N-CA-C      | -6.77 | 103.90      | 111.28   |
| 4   | S2    | 235  | LEU  | CA-C-N      | 6.76  | 126.78      | 119.89   |
| 4   | S2    | 235  | LEU  | C-N-CA      | 6.76  | 126.78      | 119.89   |
| 61  | n5    | 62   | VAL  | CA-C-N      | -6.75 | 114.82      | 123.19   |
| 61  | n5    | 62   | VAL  | C-N-CA      | -6.75 | 114.82      | 123.19   |
| 79  | q3    | 53   | GLY  | CA-C-N      | -6.75 | 114.43      | 122.93   |
| 79  | q3    | 53   | GLY  | C-N-CA      | -6.75 | 114.43      | 122.93   |
| 72  | o6    | 21   | THR  | CA-C-N      | 6.74  | 126.66      | 119.85   |
| 72  | o6    | 21   | THR  | C-N-CA      | 6.74  | 126.66      | 119.85   |
| 25  | D3    | 4    | GLY  | N-CA-C      | 6.73  | 122.70      | 114.69   |
| 57  | N1    | 71   | SER  | N-CA-C      | 6.73  | 118.03      | 108.74   |
| 12  | c0    | 88   | PRO  | N-CA-CB     | 6.71  | 110.29      | 103.25   |
| 54  | m8    | 170  | ARG  | N-CA-C      | -6.70 | 100.37      | 110.28   |
| 44  | l7    | 94   | LYS  | CA-C-N      | -6.69 | 117.03      | 122.85   |
| 44  | l7    | 94   | LYS  | C-N-CA      | -6.69 | 117.03      | 122.85   |
| 31  | D9    | 9    | SER  | N-CA-C      | 6.67  | 119.31      | 108.76   |
| 40  | L3    | 205  | VAL  | CB-CA-C     | -6.67 | 103.31      | 112.04   |
| 47  | M0    | 121  | LYS  | CA-C-N      | -6.66 | 112.90      | 119.76   |
| 47  | M0    | 121  | LYS  | C-N-CA      | -6.66 | 112.90      | 119.76   |
| 46  | l9    | 97   | PHE  | CA-C-N      | -6.66 | 113.10      | 119.76   |
| 46  | l9    | 97   | PHE  | C-N-CA      | -6.66 | 113.10      | 119.76   |
| 25  | D3    | 142  | LYS  | CA-C-N      | 6.65  | 126.41      | 119.76   |
| 25  | D3    | 142  | LYS  | C-N-CA      | 6.65  | 126.41      | 119.76   |
| 67  | o1    | 44   | MET  | N-CA-C      | 6.64  | 120.97      | 112.86   |
| 7   | s5    | 99   | MET  | N-CA-C      | 6.64  | 116.81      | 108.45   |
| 57  | n1    | 52   | MET  | N-CA-C      | 6.62  | 118.14      | 109.93   |
| 68  | o2    | 106  | VAL  | N-CA-C      | -6.59 | 104.06      | 110.72   |
| 6   | s4    | 151  | ASP  | CA-C-N      | 6.59  | 128.07      | 119.84   |
| 6   | s4    | 151  | ASP  | C-N-CA      | 6.59  | 128.07      | 119.84   |
| 36  | 1     | 92   | G    | O5'-C5'-C4' | -6.59 | 101.62      | 111.50   |
| 36  | 5     | 1152 | G    | C8-N9-C1'   | 6.58  | 146.75      | 127.00   |
| 30  | d8    | 30   | VAL  | N-CA-C      | 6.58  | 117.31      | 108.11   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56  | n0    | 134  | ASP  | N-CA-C      | -6.56 | 105.19      | 113.72   |
| 24  | d2    | 55   | ASP  | N-CA-C      | -6.56 | 101.70      | 110.55   |
| 36  | 1     | 1607 | U    | C4'-C3'-O3' | 6.55  | 119.23      | 109.40   |
| 19  | C7    | 85   | VAL  | CA-C-N      | 6.55  | 128.03      | 119.84   |
| 19  | C7    | 85   | VAL  | C-N-CA      | 6.55  | 128.03      | 119.84   |
| 44  | l7    | 191  | VAL  | CA-C-N      | -6.55 | 111.59      | 121.87   |
| 44  | l7    | 191  | VAL  | C-N-CA      | -6.55 | 111.59      | 121.87   |
| 36  | 1     | 1484 | U    | P-O3'-C3'   | 6.55  | 130.02      | 120.20   |
| 55  | M9    | 160  | GLU  | N-CA-C      | -6.54 | 104.33      | 112.90   |
| 2   | s0    | 141  | ILE  | N-CA-C      | 6.54  | 115.10      | 107.77   |
| 57  | N1    | 158  | THR  | N-CA-C      | 6.53  | 121.77      | 113.55   |
| 7   | s5    | 21   | THR  | CA-C-N      | 6.52  | 126.44      | 119.85   |
| 7   | s5    | 21   | THR  | C-N-CA      | 6.52  | 126.44      | 119.85   |
| 79  | Q3    | 78   | THR  | N-CA-C      | -6.51 | 104.27      | 111.36   |
| 71  | o5    | 41   | LEU  | CA-C-N      | 6.50  | 127.97      | 119.84   |
| 71  | o5    | 41   | LEU  | C-N-CA      | 6.50  | 127.97      | 119.84   |
| 6   | S4    | 28   | ALA  | CA-C-N      | -6.50 | 112.97      | 119.99   |
| 6   | S4    | 28   | ALA  | C-N-CA      | -6.50 | 112.97      | 119.99   |
| 50  | M4    | 30   | GLY  | N-CA-C      | -6.50 | 106.35      | 115.32   |
| 6   | s4    | 34   | GLY  | CA-C-N      | 6.50  | 126.19      | 119.56   |
| 6   | s4    | 34   | GLY  | C-N-CA      | 6.50  | 126.19      | 119.56   |
| 31  | d9    | 9    | SER  | N-CA-C      | 6.50  | 118.08      | 108.60   |
| 49  | m3    | 57   | VAL  | CB-CA-C     | -6.49 | 104.45      | 111.59   |
| 48  | m1    | 151  | SER  | N-CA-C      | -6.48 | 101.94      | 110.43   |
| 21  | C9    | 4    | VAL  | N-CA-C      | 6.47  | 118.03      | 108.65   |
| 65  | n9    | 23   | LYS  | CA-C-N      | -6.44 | 111.83      | 118.85   |
| 65  | n9    | 23   | LYS  | C-N-CA      | -6.44 | 111.83      | 118.85   |
| 64  | N8    | 115  | LYS  | CA-C-N      | -6.43 | 108.80      | 121.41   |
| 64  | N8    | 115  | LYS  | C-N-CA      | -6.43 | 108.80      | 121.41   |
| 41  | l4    | 90   | PHE  | CA-C-N      | -6.43 | 108.80      | 121.41   |
| 41  | l4    | 90   | PHE  | C-N-CA      | -6.43 | 108.80      | 121.41   |
| 4   | S2    | 233  | GLN  | CA-C-N      | -6.43 | 112.37      | 119.19   |
| 4   | S2    | 233  | GLN  | C-N-CA      | -6.43 | 112.37      | 119.19   |
| 25  | D3    | 7    | ARG  | N-CA-C      | -6.43 | 106.39      | 114.56   |
| 53  | M7    | 183  | ALA  | CA-C-O      | 6.43  | 121.67      | 117.94   |
| 33  | e1    | 87   | THR  | CA-C-N      | -6.43 | 113.05      | 119.99   |
| 33  | e1    | 87   | THR  | C-N-CA      | -6.43 | 113.05      | 119.99   |
| 11  | s9    | 172  | VAL  | N-CA-C      | -6.42 | 106.29      | 111.81   |
| 36  | 5     | 715  | A    | C4'-C3'-O3' | 6.42  | 122.63      | 113.00   |
| 40  | L3    | 186  | GLY  | N-CA-C      | 6.42  | 128.39      | 113.18   |
| 5   | S3    | 219  | ALA  | CA-C-N      | 6.41  | 127.86      | 119.84   |
| 5   | S3    | 219  | ALA  | C-N-CA      | 6.41  | 127.86      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 64  | N8    | 95   | SER  | N-CA-C      | 6.41  | 118.82      | 109.07   |
| 36  | 5     | 1879 | A    | O5'-P-OP1   | 6.41  | 127.24      | 108.00   |
| 36  | 1     | 1117 | G    | O5'-P-OP1   | -6.41 | 88.78       | 108.00   |
| 47  | m0    | 131  | ILE  | CB-CA-C     | -6.38 | 104.39      | 111.35   |
| 34  | SR    | 157  | VAL  | N-CA-C      | 6.35  | 114.17      | 107.76   |
| 54  | m8    | 99   | THR  | N-CA-C      | 6.33  | 124.29      | 110.80   |
| 40  | l3    | 169  | THR  | CA-C-N      | -6.33 | 113.43      | 120.45   |
| 40  | l3    | 169  | THR  | C-N-CA      | -6.33 | 113.43      | 120.45   |
| 41  | L4    | 328  | ASN  | N-CA-C      | 6.31  | 123.75      | 109.81   |
| 43  | l6    | 66   | SER  | CA-C-N      | -6.30 | 111.98      | 121.87   |
| 43  | l6    | 66   | SER  | C-N-CA      | -6.30 | 111.98      | 121.87   |
| 7   | S5    | 66   | GLN  | CA-C-N      | 6.29  | 126.48      | 120.31   |
| 7   | S5    | 66   | GLN  | C-N-CA      | 6.29  | 126.48      | 120.31   |
| 41  | L4    | 192  | GLY  | N-CA-C      | -6.29 | 105.01      | 113.24   |
| 41  | l4    | 14   | GLU  | N-CA-C      | 6.28  | 119.14      | 110.35   |
| 18  | C6    | 43   | ILE  | N-CA-C      | -6.27 | 104.54      | 113.07   |
| 25  | D3    | 111  | GLY  | N-CA-C      | -6.26 | 100.37      | 112.02   |
| 23  | D1    | 13   | VAL  | CA-C-N      | 6.25  | 126.27      | 119.89   |
| 23  | D1    | 13   | VAL  | C-N-CA      | 6.25  | 126.27      | 119.89   |
| 33  | E1    | 138  | ARG  | N-CA-C      | 6.25  | 124.11      | 110.80   |
| 56  | n0    | 132  | THR  | N-CA-C      | -6.24 | 101.86      | 110.35   |
| 71  | O5    | 119  | LYS  | N-CA-C      | -6.24 | 97.52       | 110.80   |
| 40  | l3    | 186  | GLY  | N-CA-C      | 6.23  | 121.42      | 111.64   |
| 36  | 1     | 282  | G    | C2'-C3'-O3' | 6.21  | 123.02      | 113.70   |
| 47  | M0    | 189  | GLU  | N-CA-C      | 6.21  | 124.03      | 110.80   |
| 3   | s1    | 22   | ASP  | CA-C-N      | 6.21  | 125.90      | 119.56   |
| 3   | s1    | 22   | ASP  | C-N-CA      | 6.21  | 125.90      | 119.56   |
| 20  | c8    | 102  | ALA  | CB-CA-C     | -6.21 | 109.42      | 116.63   |
| 44  | l7    | 221  | LYS  | N-CA-C      | -6.21 | 99.86       | 109.24   |
| 2   | S0    | 108  | THR  | N-CA-C      | -6.20 | 102.19      | 110.55   |
| 68  | o2    | 124  | GLY  | CA-C-N      | -6.20 | 113.19      | 122.24   |
| 68  | o2    | 124  | GLY  | C-N-CA      | -6.20 | 113.19      | 122.24   |
| 36  | 1     | 1103 | A    | O3'-P-O5'   | -6.18 | 94.73       | 104.00   |
| 29  | D7    | 37   | CYS  | CA-C-N      | 6.17  | 127.56      | 119.84   |
| 29  | D7    | 37   | CYS  | C-N-CA      | 6.17  | 127.56      | 119.84   |
| 56  | N0    | 155  | ARG  | CA-C-N      | -6.17 | 114.86      | 123.13   |
| 56  | N0    | 155  | ARG  | C-N-CA      | -6.17 | 114.86      | 123.13   |
| 61  | N5    | 49   | LYS  | N-CA-C      | 6.17  | 121.84      | 113.21   |
| 72  | O6    | 21   | THR  | CA-C-N      | 6.16  | 126.08      | 119.85   |
| 72  | O6    | 21   | THR  | C-N-CA      | 6.16  | 126.08      | 119.85   |
| 60  | n4    | 75   | THR  | N-CA-C      | 6.16  | 117.88      | 108.52   |
| 61  | N5    | 43   | ALA  | CA-C-N      | 6.16  | 127.54      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 61  | N5    | 43   | ALA  | C-N-CA      | 6.16  | 127.54      | 119.84   |
| 36  | 1     | 715  | A    | C4'-C3'-O3' | 6.15  | 122.23      | 113.00   |
| 62  | n6    | 56   | VAL  | N-CA-C      | 6.15  | 117.55      | 108.45   |
| 36  | 5     | 1152 | G    | C4-N9-C1'   | -6.15 | 108.06      | 126.50   |
| 67  | o1    | 94   | GLU  | CA-C-N      | -6.15 | 114.44      | 120.52   |
| 67  | o1    | 94   | GLU  | C-N-CA      | -6.15 | 114.44      | 120.52   |
| 65  | N9    | 12   | GLN  | N-CA-C      | 6.14  | 117.97      | 111.28   |
| 16  | c4    | 35   | GLY  | N-CA-C      | 6.13  | 127.72      | 113.18   |
| 60  | n4    | 84   | GLY  | N-CA-C      | -6.13 | 106.95      | 114.92   |
| 49  | M3    | 26   | PHE  | N-CA-C      | -6.13 | 105.06      | 112.54   |
| 52  | m6    | 110  | PRO  | CA-C-O      | -6.11 | 111.69      | 120.56   |
| 56  | n0    | 171  | PHE  | N-CA-C      | 6.11  | 120.59      | 113.20   |
| 69  | O3    | 26   | ASN  | N-CA-C      | 6.11  | 119.99      | 112.54   |
| 41  | l4    | 49   | ALA  | N-CA-C      | 6.11  | 119.46      | 110.30   |
| 15  | C3    | 28   | LEU  | CB-CA-C     | -6.11 | 108.52      | 115.79   |
| 12  | c0    | 3    | MET  | CA-C-N      | 6.10  | 126.29      | 120.31   |
| 12  | c0    | 3    | MET  | C-N-CA      | 6.10  | 126.29      | 120.31   |
| 65  | n9    | 20   | GLY  | O-C-N       | 6.10  | 128.74      | 123.25   |
| 40  | l3    | 95   | THR  | CA-C-N      | -6.09 | 112.23      | 119.84   |
| 40  | l3    | 95   | THR  | C-N-CA      | -6.09 | 112.23      | 119.84   |
| 36  | 1     | 1484 | U    | C2'-C3'-O3' | 6.09  | 118.63      | 109.50   |
| 36  | 1     | 2513 | U    | C4'-C3'-O3' | 6.09  | 118.53      | 109.40   |
| 48  | M1    | 23   | VAL  | N-CA-C      | 6.09  | 112.72      | 106.21   |
| 68  | O2    | 42   | VAL  | N-CA-C      | -6.08 | 104.92      | 110.82   |
| 2   | s0    | 9    | LEU  | N-CA-C      | 6.08  | 118.41      | 111.11   |
| 64  | n8    | 67   | HIS  | N-CA-C      | -6.08 | 103.97      | 111.33   |
| 46  | L9    | 126  | VAL  | CA-C-N      | -6.08 | 113.71      | 119.85   |
| 46  | L9    | 126  | VAL  | C-N-CA      | -6.08 | 113.71      | 119.85   |
| 1   | 2     | 1339 | C    | P-O3'-C3'   | 6.08  | 129.32      | 120.20   |
| 68  | o2    | 67   | SER  | CA-C-N      | -6.08 | 112.59      | 119.28   |
| 68  | o2    | 67   | SER  | C-N-CA      | -6.08 | 112.59      | 119.28   |
| 42  | L5    | 93   | THR  | N-CA-C      | -6.08 | 105.17      | 114.16   |
| 17  | c5    | 124  | THR  | CA-C-N      | 6.07  | 127.42      | 119.84   |
| 17  | c5    | 124  | THR  | C-N-CA      | 6.07  | 127.42      | 119.84   |
| 18  | c6    | 63   | ILE  | N-CA-C      | 6.06  | 116.35      | 108.35   |
| 56  | N0    | 19   | VAL  | CA-C-N      | -6.05 | 113.74      | 119.85   |
| 56  | N0    | 19   | VAL  | C-N-CA      | -6.05 | 113.74      | 119.85   |
| 33  | e1    | 129  | GLY  | N-CA-C      | -6.05 | 106.58      | 115.72   |
| 39  | L2    | 232  | GLY  | N-CA-C      | -6.05 | 106.68      | 114.85   |
| 53  | M7    | 140  | GLU  | N-CA-C      | 6.05  | 119.40      | 109.72   |
| 57  | N1    | 140  | ILE  | CA-C-N      | -6.03 | 115.33      | 122.93   |
| 57  | N1    | 140  | ILE  | C-N-CA      | -6.03 | 115.33      | 122.93   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | s9    | 159  | ALA  | CA-C-N      | 6.03  | 125.91      | 119.28   |
| 11  | s9    | 159  | ALA  | C-N-CA      | 6.03  | 125.91      | 119.28   |
| 70  | O4    | 11   | ASN  | CA-C-N      | 6.03  | 127.37      | 119.84   |
| 70  | O4    | 11   | ASN  | C-N-CA      | 6.03  | 127.37      | 119.84   |
| 70  | O4    | 51   | LEU  | CA-CB-CG    | 6.01  | 137.35      | 116.30   |
| 41  | l4    | 222  | VAL  | CA-C-N      | 6.01  | 127.36      | 119.84   |
| 41  | l4    | 222  | VAL  | C-N-CA      | 6.01  | 127.36      | 119.84   |
| 8   | S6    | 60   | GLY  | N-CA-C      | 6.01  | 123.96      | 115.30   |
| 39  | l2    | 118  | GLU  | N-CA-C      | -6.00 | 106.50      | 113.88   |
| 56  | N0    | 23   | LYS  | N-CA-C      | 5.99  | 118.77      | 111.82   |
| 1   | 6     | 103  | A    | C4'-C3'-O3' | 5.99  | 118.38      | 109.40   |
| 13  | C1    | 58   | CYS  | CA-C-N      | 5.99  | 125.67      | 119.56   |
| 13  | C1    | 58   | CYS  | C-N-CA      | 5.99  | 125.67      | 119.56   |
| 71  | O5    | 41   | LEU  | CA-C-N      | 5.98  | 125.86      | 119.28   |
| 71  | O5    | 41   | LEU  | C-N-CA      | 5.98  | 125.86      | 119.28   |
| 33  | E1    | 102  | VAL  | N-CA-C      | 5.98  | 121.78      | 109.34   |
| 77  | q1    | 24   | SER  | N-CA-C      | -5.98 | 105.84      | 113.02   |
| 19  | C7    | 54   | THR  | N-CA-C      | -5.98 | 105.25      | 112.54   |
| 6   | S4    | 103  | TYR  | N-CA-C      | 5.97  | 118.62      | 110.55   |
| 58  | N2    | 59   | ASP  | N-CA-C      | -5.97 | 105.97      | 113.20   |
| 24  | d2    | 97   | ARG  | CA-C-N      | -5.97 | 113.11      | 122.49   |
| 24  | d2    | 97   | ARG  | C-N-CA      | -5.97 | 113.11      | 122.49   |
| 8   | s6    | 134  | GLY  | CA-C-N      | 5.97  | 125.91      | 119.76   |
| 8   | s6    | 134  | GLY  | C-N-CA      | 5.97  | 125.91      | 119.76   |
| 42  | l5    | 23   | ARG  | N-CA-C      | -5.97 | 104.12      | 111.40   |
| 68  | O2    | 40   | SER  | N-CA-C      | 5.95  | 119.11      | 110.42   |
| 36  | 1     | 112  | U    | N1-C1'-C2'  | -5.95 | 105.07      | 114.00   |
| 39  | L2    | 156  | LYS  | CA-C-N      | -5.95 | 115.43      | 122.93   |
| 39  | L2    | 156  | LYS  | C-N-CA      | -5.95 | 115.43      | 122.93   |
| 56  | n0    | 68   | HIS  | CA-C-N      | 5.94  | 127.27      | 119.84   |
| 56  | n0    | 68   | HIS  | C-N-CA      | 5.94  | 127.27      | 119.84   |
| 56  | N0    | 134  | ASP  | N-CA-C      | -5.94 | 106.07      | 113.38   |
| 40  | l3    | 253  | GLY  | N-CA-C      | 5.94  | 118.99      | 111.09   |
| 33  | E1    | 104  | SER  | N-CA-C      | -5.93 | 106.04      | 113.28   |
| 11  | S9    | 143  | ILE  | CA-C-N      | 5.93  | 125.61      | 119.56   |
| 11  | S9    | 143  | ILE  | C-N-CA      | 5.93  | 125.61      | 119.56   |
| 19  | c7    | 64   | GLY  | CA-C-N      | 5.93  | 127.25      | 119.84   |
| 19  | c7    | 64   | GLY  | C-N-CA      | 5.93  | 127.25      | 119.84   |
| 51  | m5    | 90   | ASN  | CA-C-N      | -5.93 | 113.12      | 122.79   |
| 51  | m5    | 90   | ASN  | C-N-CA      | -5.93 | 113.12      | 122.79   |
| 53  | M7    | 183  | ALA  | N-CA-C      | 5.91  | 113.63      | 108.78   |
| 36  | 1     | 1607 | U    | P-O3'-C3'   | 5.91  | 129.06      | 120.20   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 46  | l9    | 151 | VAL  | CB-CA-C     | -5.90 | 104.31      | 112.04   |
| 59  | n3    | 50  | PRO  | CA-C-O      | -5.90 | 114.62      | 121.34   |
| 15  | c3    | 81  | ALA  | CA-C-N      | 5.90  | 125.87      | 120.21   |
| 15  | c3    | 81  | ALA  | C-N-CA      | 5.90  | 125.87      | 120.21   |
| 54  | m8    | 96  | PHE  | CA-C-N      | 5.90  | 127.21      | 119.84   |
| 54  | m8    | 96  | PHE  | C-N-CA      | 5.90  | 127.21      | 119.84   |
| 62  | N6    | 4   | GLN  | N-CA-C      | -5.89 | 107.32      | 114.75   |
| 64  | N8    | 46  | ASP  | N-CA-C      | -5.89 | 102.33      | 110.35   |
| 76  | Q0    | 79  | GLU  | CA-C-N      | 5.89  | 127.20      | 119.84   |
| 76  | Q0    | 79  | GLU  | C-N-CA      | 5.89  | 127.20      | 119.84   |
| 41  | l4    | 230 | VAL  | CB-CA-C     | -5.89 | 104.09      | 112.22   |
| 44  | l7    | 76  | TYR  | CA-C-N      | -5.89 | 115.27      | 123.10   |
| 44  | l7    | 76  | TYR  | C-N-CA      | -5.89 | 115.27      | 123.10   |
| 21  | c9    | 126 | GLU  | N-CA-C      | -5.89 | 104.99      | 111.82   |
| 43  | L6    | 88  | SER  | CA-C-N      | -5.88 | 114.61      | 122.72   |
| 43  | L6    | 88  | SER  | C-N-CA      | -5.88 | 114.61      | 122.72   |
| 41  | L4    | 191 | LYS  | N-CA-C      | -5.88 | 106.20      | 113.19   |
| 79  | Q3    | 71  | VAL  | CB-CA-C     | -5.87 | 104.34      | 112.04   |
| 45  | l8    | 72  | PRO  | CA-C-N      | 5.87  | 126.28      | 119.47   |
| 45  | l8    | 72  | PRO  | C-N-CA      | 5.87  | 126.28      | 119.47   |
| 39  | l2    | 207 | VAL  | CB-CA-C     | -5.87 | 103.07      | 112.16   |
| 12  | C0    | 82  | LEU  | CA-C-N      | 5.85  | 125.79      | 119.76   |
| 12  | C0    | 82  | LEU  | C-N-CA      | 5.85  | 125.79      | 119.76   |
| 36  | 5     | 398 | A    | O5'-P-OP2   | -5.85 | 90.44       | 108.00   |
| 39  | L2    | 207 | VAL  | CB-CA-C     | -5.85 | 101.70      | 111.29   |
| 41  | l4    | 192 | GLY  | N-CA-C      | -5.84 | 107.09      | 114.16   |
| 40  | L3    | 241 | LYS  | CA-C-N      | -5.84 | 113.15      | 121.50   |
| 40  | L3    | 241 | LYS  | C-N-CA      | -5.84 | 113.15      | 121.50   |
| 51  | m5    | 61  | ILE  | N-CA-C      | 5.84  | 116.27      | 107.80   |
| 49  | m3    | 46  | ILE  | N-CA-C      | -5.84 | 106.09      | 112.80   |
| 49  | M3    | 63  | VAL  | CB-CA-C     | -5.82 | 101.74      | 111.29   |
| 1   | 6     | 158 | U    | C2'-C3'-O3' | 5.82  | 118.23      | 109.50   |
| 52  | M6    | 146 | GLY  | N-CA-C      | 5.82  | 121.40      | 114.48   |
| 58  | n2    | 21  | SER  | CA-C-N      | -5.81 | 113.69      | 119.56   |
| 58  | n2    | 21  | SER  | C-N-CA      | -5.81 | 113.69      | 119.56   |
| 8   | s6    | 129 | VAL  | CA-C-N      | 5.81  | 125.72      | 119.85   |
| 8   | s6    | 129 | VAL  | C-N-CA      | 5.81  | 125.72      | 119.85   |
| 67  | o1    | 46  | THR  | N-CA-C      | 5.81  | 117.41      | 111.14   |
| 16  | c4    | 80  | HIS  | CA-C-N      | -5.81 | 115.99      | 123.19   |
| 16  | c4    | 80  | HIS  | C-N-CA      | -5.81 | 115.99      | 123.19   |
| 55  | M9    | 41  | ILE  | N-CA-C      | -5.80 | 105.43      | 111.58   |
| 42  | L5    | 24  | ARG  | N-CA-C      | -5.80 | 105.09      | 111.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 64  | n8    | 125  | VAL  | N-CA-C      | 5.79  | 116.14      | 107.51   |
| 64  | N8    | 116  | GLY  | N-CA-C      | 5.79  | 126.91      | 113.18   |
| 33  | e1    | 147  | VAL  | N-CA-C      | 5.79  | 117.18      | 109.37   |
| 66  | O0    | 32   | LYS  | N-CA-C      | -5.78 | 104.97      | 111.28   |
| 63  | N7    | 81   | LEU  | CA-C-N      | -5.78 | 113.81      | 119.76   |
| 63  | N7    | 81   | LEU  | C-N-CA      | -5.78 | 113.81      | 119.76   |
| 41  | l4    | 328  | ASN  | N-CA-C      | 5.78  | 122.58      | 109.81   |
| 12  | C0    | 87   | VAL  | CA-C-N      | 5.77  | 127.06      | 119.84   |
| 12  | C0    | 87   | VAL  | C-N-CA      | 5.77  | 127.06      | 119.84   |
| 65  | n9    | 39   | PHE  | N-CA-CB     | 5.77  | 120.24      | 110.49   |
| 44  | L7    | 164  | SER  | N-CA-C      | 5.76  | 123.08      | 110.80   |
| 64  | n8    | 52   | TYR  | N-CA-C      | 5.76  | 117.25      | 110.97   |
| 14  | c2    | 130  | THR  | CB-CA-C     | -5.76 | 108.94      | 115.79   |
| 71  | o5    | 119  | LYS  | N-CA-C      | -5.75 | 98.56       | 110.80   |
| 31  | D9    | 36   | LEU  | CA-CB-CG    | 5.74  | 136.39      | 116.30   |
| 56  | n0    | 116  | ALA  | N-CA-C      | 5.74  | 117.41      | 109.15   |
| 44  | L7    | 93   | ASN  | N-CA-C      | 5.74  | 119.01      | 110.52   |
| 35  | sM    | 49   | LYS  | N-CA-C      | -5.74 | 106.44      | 113.50   |
| 2   | S0    | 166  | GLY  | N-CA-C      | 5.73  | 117.35      | 111.56   |
| 11  | S9    | 152  | SER  | N-CA-C      | -5.73 | 105.93      | 114.64   |
| 44  | l7    | 160  | ARG  | CA-C-N      | -5.72 | 118.35      | 123.33   |
| 44  | l7    | 160  | ARG  | C-N-CA      | -5.72 | 118.35      | 123.33   |
| 16  | C4    | 91   | THR  | N-CA-C      | 5.72  | 118.25      | 111.33   |
| 40  | l3    | 114  | VAL  | CB-CA-C     | -5.72 | 104.33      | 112.22   |
| 44  | L7    | 159  | GLN  | N-CA-C      | 5.71  | 119.83      | 112.86   |
| 57  | n1    | 149  | GLN  | CA-C-N      | -5.71 | 114.66      | 122.93   |
| 57  | n1    | 149  | GLN  | C-N-CA      | -5.71 | 114.66      | 122.93   |
| 65  | n9    | 20   | GLY  | CA-C-N      | 5.71  | 132.24      | 121.97   |
| 65  | n9    | 20   | GLY  | C-N-CA      | 5.71  | 132.24      | 121.97   |
| 47  | M0    | 32   | ARG  | CA-C-N      | -5.70 | 115.75      | 122.93   |
| 47  | M0    | 32   | ARG  | C-N-CA      | -5.70 | 115.75      | 122.93   |
| 56  | N0    | 132  | THR  | N-CA-C      | -5.69 | 102.61      | 110.35   |
| 64  | n8    | 42   | ARG  | N-CA-C      | 5.68  | 117.47      | 111.28   |
| 2   | S0    | 186  | GLY  | N-CA-C      | 5.68  | 121.46      | 110.66   |
| 44  | L7    | 119  | VAL  | N-CA-C      | 5.68  | 116.56      | 107.98   |
| 36  | 1     | 1716 | U    | C2'-C3'-O3' | 5.68  | 118.01      | 109.50   |
| 36  | 5     | 406  | G    | O4'-C1'-N9  | 5.67  | 116.71      | 108.20   |
| 71  | O5    | 80   | LEU  | N-CA-C      | -5.67 | 105.30      | 114.09   |
| 41  | l4    | 145  | ILE  | CA-C-N      | 5.67  | 126.92      | 119.84   |
| 41  | l4    | 145  | ILE  | C-N-CA      | 5.67  | 126.92      | 119.84   |
| 55  | m9    | 151  | ARG  | N-CA-C      | -5.67 | 106.33      | 113.18   |
| 2   | S0    | 167  | LYS  | CB-CA-C     | -5.66 | 110.06      | 116.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | M3    | 85   | LEU  | CA-CB-CG    | 5.66  | 136.10      | 116.30   |
| 1   | 6     | 1097 | U    | C2'-C3'-O3' | 5.65  | 117.97      | 109.50   |
| 25  | D3    | 129  | GLY  | CA-C-N      | -5.64 | 117.18      | 123.16   |
| 25  | D3    | 129  | GLY  | C-N-CA      | -5.64 | 117.18      | 123.16   |
| 6   | s4    | 167  | GLY  | N-CA-C      | -5.64 | 101.76      | 111.47   |
| 73  | O7    | 87   | SER  | N-CA-C      | 5.64  | 115.83      | 107.88   |
| 33  | E1    | 144  | CYS  | N-CA-C      | -5.63 | 98.81       | 110.80   |
| 61  | n5    | 56   | ARG  | N-CA-C      | -5.62 | 102.57      | 110.50   |
| 44  | l7    | 119  | VAL  | CB-CA-C     | -5.62 | 105.16      | 111.23   |
| 65  | N9    | 20   | GLY  | N-CA-C      | 5.62  | 126.50      | 113.18   |
| 71  | o5    | 70   | TYR  | N-CA-C      | -5.62 | 105.84      | 114.16   |
| 50  | m4    | 53   | VAL  | CA-C-N      | 5.62  | 125.80      | 119.90   |
| 50  | m4    | 53   | VAL  | C-N-CA      | 5.62  | 125.80      | 119.90   |
| 40  | l3    | 19   | ARG  | NE-CZ-NH2   | -5.62 | 114.15      | 119.20   |
| 46  | L9    | 41   | ILE  | N-CA-C      | 5.61  | 121.01      | 109.34   |
| 55  | m9    | 125  | LYS  | N-CA-C      | -5.61 | 104.79      | 111.69   |
| 53  | M7    | 10   | ASN  | CA-C-N      | -5.61 | 113.84      | 119.56   |
| 53  | M7    | 10   | ASN  | C-N-CA      | -5.61 | 113.84      | 119.56   |
| 44  | L7    | 131  | GLU  | CA-C-N      | -5.59 | 113.91      | 120.12   |
| 44  | L7    | 131  | GLU  | C-N-CA      | -5.59 | 113.91      | 120.12   |
| 36  | 1     | 637  | C    | O3'-P-O5'   | 5.59  | 112.39      | 104.00   |
| 67  | o1    | 64   | VAL  | CB-CA-C     | -5.59 | 103.89      | 112.05   |
| 9   | S7    | 50   | ASP  | N-CA-C      | 5.58  | 118.67      | 109.85   |
| 26  | D4    | 86   | GLU  | CA-C-N      | 5.58  | 125.60      | 119.90   |
| 26  | D4    | 86   | GLU  | C-N-CA      | 5.58  | 125.60      | 119.90   |
| 59  | n3    | 17   | LEU  | CA-C-N      | 5.58  | 125.53      | 119.78   |
| 59  | n3    | 17   | LEU  | C-N-CA      | 5.58  | 125.53      | 119.78   |
| 11  | s9    | 19   | TYR  | N-CA-C      | 5.58  | 116.41      | 108.54   |
| 35  | sM    | 43   | ASP  | CA-C-N      | 5.58  | 125.19      | 119.56   |
| 35  | sM    | 43   | ASP  | C-N-CA      | 5.58  | 125.19      | 119.56   |
| 1   | 2     | 158  | U    | C2'-C3'-O3' | 5.57  | 117.86      | 109.50   |
| 36  | 1     | 637  | C    | OP2-P-O3'   | -5.57 | 91.28       | 108.00   |
| 49  | m3    | 100  | ARG  | N-CA-C      | -5.57 | 101.10      | 109.79   |
| 18  | c6    | 114  | ARG  | N-CA-C      | -5.56 | 102.95      | 110.68   |
| 33  | e1    | 104  | SER  | N-CA-C      | -5.55 | 106.49      | 113.20   |
| 56  | n0    | 165  | TYR  | N-CA-C      | -5.55 | 105.82      | 112.59   |
| 36  | 5     | 2249 | G    | C2'-C3'-O3' | 5.54  | 122.02      | 113.70   |
| 54  | M8    | 99   | THR  | CB-CA-C     | -5.54 | 99.40       | 110.42   |
| 59  | N3    | 114  | ILE  | CA-C-N      | -5.53 | 115.09      | 122.72   |
| 59  | N3    | 114  | ILE  | C-N-CA      | -5.53 | 115.09      | 122.72   |
| 17  | C5    | 52   | LYS  | CA-C-N      | -5.53 | 116.06      | 121.65   |
| 17  | C5    | 52   | LYS  | C-N-CA      | -5.53 | 116.06      | 121.65   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | s9    | 124  | HIS  | N-CA-C      | -5.53 | 105.15      | 111.07   |
| 25  | d3    | 5    | LYS  | CA-C-N      | -5.53 | 115.05      | 120.52   |
| 25  | d3    | 5    | LYS  | C-N-CA      | -5.53 | 115.05      | 120.52   |
| 53  | m7    | 118  | GLN  | CA-C-N      | -5.53 | 116.34      | 123.19   |
| 53  | m7    | 118  | GLN  | C-N-CA      | -5.53 | 116.34      | 123.19   |
| 7   | s5    | 29   | ILE  | CA-C-N      | 5.52  | 125.43      | 119.85   |
| 7   | s5    | 29   | ILE  | C-N-CA      | 5.52  | 125.43      | 119.85   |
| 39  | L2    | 25   | GLY  | N-CA-C      | -5.52 | 106.50      | 112.08   |
| 1   | 2     | 1196 | A    | C4'-C3'-O3' | 5.52  | 117.68      | 109.40   |
| 44  | l7    | 229  | PHE  | CA-CB-CG    | 5.52  | 119.32      | 113.80   |
| 45  | L8    | 70   | LYS  | CA-C-N      | -5.52 | 117.36      | 123.43   |
| 45  | L8    | 70   | LYS  | C-N-CA      | -5.52 | 117.36      | 123.43   |
| 48  | m1    | 73   | GLY  | CA-C-N      | 5.51  | 125.87      | 119.47   |
| 48  | m1    | 73   | GLY  | C-N-CA      | 5.51  | 125.87      | 119.47   |
| 40  | L3    | 316  | GLU  | N-CA-C      | 5.51  | 121.42      | 114.31   |
| 47  | m0    | 121  | LYS  | CA-C-N      | -5.51 | 114.08      | 119.76   |
| 47  | m0    | 121  | LYS  | C-N-CA      | -5.51 | 114.08      | 119.76   |
| 11  | S9    | 138  | LYS  | N-CA-C      | -5.50 | 106.34      | 113.16   |
| 20  | C8    | 102  | ALA  | CB-CA-C     | -5.50 | 110.25      | 116.63   |
| 48  | m1    | 127  | PHE  | CA-C-N      | -5.50 | 115.24      | 122.99   |
| 48  | m1    | 127  | PHE  | C-N-CA      | -5.50 | 115.24      | 122.99   |
| 52  | m6    | 85   | ARG  | N-CA-C      | -5.50 | 105.45      | 111.82   |
| 33  | e1    | 123  | ASN  | CA-C-N      | 5.49  | 126.70      | 119.84   |
| 33  | e1    | 123  | ASN  | C-N-CA      | 5.49  | 126.70      | 119.84   |
| 41  | l4    | 73   | ARG  | CB-CG-CD    | -5.48 | 98.69       | 111.30   |
| 36  | 1     | 637  | C    | O4'-C1'-N1  | 5.48  | 116.72      | 108.50   |
| 69  | o3    | 86   | ARG  | N-CA-C      | -5.47 | 105.31      | 111.28   |
| 9   | S7    | 97   | ARG  | N-CA-C      | 5.47  | 118.42      | 111.69   |
| 9   | s7    | 9    | LEU  | O-C-N       | 5.47  | 124.88      | 120.83   |
| 64  | N8    | 118  | ILE  | CA-C-N      | -5.47 | 114.96      | 120.21   |
| 64  | N8    | 118  | ILE  | C-N-CA      | -5.47 | 114.96      | 120.21   |
| 43  | L6    | 130  | ILE  | N-CA-C      | 5.46  | 116.62      | 108.54   |
| 42  | l5    | 182  | GLY  | N-CA-C      | -5.46 | 107.25      | 114.95   |
| 40  | L3    | 278  | ILE  | N-CA-C      | 5.46  | 116.71      | 108.96   |
| 41  | L4    | 194  | TYR  | CA-CB-CG    | 5.46  | 123.73      | 113.90   |
| 6   | s4    | 13   | ALA  | N-CA-C      | -5.46 | 106.30      | 113.17   |
| 73  | o7    | 5    | THR  | CA-C-N      | -5.45 | 113.02      | 119.84   |
| 73  | o7    | 5    | THR  | C-N-CA      | -5.45 | 113.02      | 119.84   |
| 36  | 1     | 895  | A    | N9-C1'-C2'  | 5.45  | 120.17      | 112.00   |
| 51  | M5    | 153  | ASP  | CA-C-N      | -5.44 | 114.01      | 119.56   |
| 51  | M5    | 153  | ASP  | C-N-CA      | -5.44 | 114.01      | 119.56   |
| 2   | s0    | 77   | SER  | N-CA-C      | 5.44  | 116.90      | 107.93   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 6     | 66   | U    | C4'-C3'-O3' | 5.44  | 117.55      | 109.40   |
| 16  | c4    | 95   | GLY  | CA-C-N      | 5.43  | 125.52      | 119.32   |
| 16  | c4    | 95   | GLY  | C-N-CA      | 5.43  | 125.52      | 119.32   |
| 30  | d8    | 53   | ILE  | N-CA-C      | 5.43  | 116.30      | 108.48   |
| 25  | d3    | 130  | VAL  | CB-CA-C     | -5.43 | 106.09      | 111.30   |
| 20  | C8    | 109  | LEU  | N-CA-C      | -5.43 | 105.36      | 111.28   |
| 36  | 5     | 2404 | A    | N9-C1'-C2'  | -5.42 | 103.87      | 112.00   |
| 36  | 5     | 2513 | U    | C4'-C3'-O3' | 5.42  | 117.53      | 109.40   |
| 29  | D7    | 50   | ALA  | N-CA-C      | 5.42  | 117.26      | 111.36   |
| 27  | D5    | 98   | GLN  | N-CA-C      | 5.41  | 117.16      | 107.80   |
| 11  | s9    | 66   | ASP  | CA-C-N      | 5.41  | 125.23      | 119.28   |
| 11  | s9    | 66   | ASP  | C-N-CA      | 5.41  | 125.23      | 119.28   |
| 49  | m3    | 141  | ALA  | N-CA-C      | -5.41 | 99.28       | 110.80   |
| 68  | o2    | 4    | LEU  | CA-C-N      | 5.41  | 126.60      | 119.84   |
| 68  | o2    | 4    | LEU  | C-N-CA      | 5.41  | 126.60      | 119.84   |
| 62  | n6    | 68   | GLY  | N-CA-C      | 5.41  | 118.36      | 110.63   |
| 45  | l8    | 68   | ARG  | N-CA-C      | -5.41 | 103.36      | 110.33   |
| 41  | l4    | 239  | ALA  | CA-C-N      | -5.40 | 114.40      | 119.85   |
| 41  | l4    | 239  | ALA  | C-N-CA      | -5.40 | 114.40      | 119.85   |
| 64  | n8    | 46   | ASP  | CA-C-O      | -5.40 | 115.67      | 121.56   |
| 24  | d2    | 102  | VAL  | CA-C-N      | -5.40 | 115.44      | 122.94   |
| 24  | d2    | 102  | VAL  | C-N-CA      | -5.40 | 115.44      | 122.94   |
| 36  | 1     | 2513 | U    | N1-C1'-C2'  | -5.39 | 105.91      | 114.00   |
| 7   | s5    | 79   | ASN  | N-CA-C      | 5.39  | 117.24      | 111.36   |
| 39  | l2    | 238  | ILE  | O-C-N       | -5.39 | 115.83      | 122.57   |
| 40  | l3    | 19   | ARG  | CG-CD-NE    | -5.39 | 100.13      | 112.00   |
| 49  | M3    | 165  | SER  | N-CA-C      | 5.39  | 117.25      | 110.24   |
| 45  | l8    | 232  | HIS  | N-CA-C      | 5.39  | 117.69      | 108.90   |
| 49  | M3    | 55   | ARG  | CA-C-N      | 5.39  | 125.86      | 120.52   |
| 49  | M3    | 55   | ARG  | C-N-CA      | 5.39  | 125.86      | 120.52   |
| 54  | m8    | 99   | THR  | CB-CA-C     | -5.39 | 99.69       | 110.42   |
| 36  | 5     | 1307 | G    | P-O3'-C3'   | 5.38  | 128.26      | 120.20   |
| 12  | C0    | 77   | ARG  | N-CA-C      | -5.37 | 105.59      | 111.82   |
| 7   | s5    | 44   | ASN  | N-CA-C      | -5.37 | 104.66      | 111.11   |
| 36  | 5     | 2524 | A    | N9-C1'-C2'  | 5.37  | 122.06      | 114.00   |
| 64  | n8    | 15   | VAL  | CA-C-N      | -5.37 | 115.73      | 125.66   |
| 64  | n8    | 15   | VAL  | C-N-CA      | -5.37 | 115.73      | 125.66   |
| 76  | Q0    | 100  | TYR  | N-CA-C      | 5.36  | 119.40      | 112.86   |
| 44  | l7    | 227  | GLY  | N-CA-C      | 5.36  | 125.89      | 113.18   |
| 3   | s1    | 131  | ASP  | N-CA-C      | -5.36 | 103.62      | 110.53   |
| 64  | n8    | 8    | THR  | N-CA-C      | -5.36 | 106.00      | 112.54   |
| 62  | N6    | 7    | ASP  | CA-C-N      | -5.36 | 116.19      | 123.10   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 62  | N6    | 7    | ASP  | C-N-CA     | -5.36 | 116.19      | 123.10   |
| 52  | M6    | 79   | ILE  | N-CA-C     | -5.35 | 105.17      | 110.62   |
| 4   | s2    | 107  | SER  | N-CA-C     | -5.34 | 99.43       | 110.80   |
| 64  | n8    | 82   | ILE  | CA-C-N     | -5.34 | 114.46      | 119.85   |
| 64  | n8    | 82   | ILE  | C-N-CA     | -5.34 | 114.46      | 119.85   |
| 53  | M7    | 173  | ARG  | N-CA-C     | -5.33 | 106.82      | 113.38   |
| 40  | l3    | 241  | LYS  | CA-C-N     | -5.33 | 114.68      | 122.19   |
| 40  | l3    | 241  | LYS  | C-N-CA     | -5.33 | 114.68      | 122.19   |
| 60  | n4    | 76   | VAL  | N-CA-C     | 5.33  | 120.42      | 109.34   |
| 48  | M1    | 10   | ARG  | N-CA-C     | -5.33 | 105.48      | 112.72   |
| 73  | O7    | 58   | THR  | N-CA-CB    | 5.32  | 117.67      | 110.38   |
| 58  | n2    | 103  | TYR  | N-CA-C     | 5.32  | 117.33      | 108.02   |
| 15  | C3    | 69   | ASN  | N-CA-C     | 5.32  | 117.76      | 109.52   |
| 1   | 2     | 1761 | U    | P-O3'-C3'  | 5.31  | 128.16      | 120.20   |
| 41  | l4    | 221  | ASN  | CA-C-N     | -5.31 | 117.50      | 123.02   |
| 41  | l4    | 221  | ASN  | C-N-CA     | -5.31 | 117.50      | 123.02   |
| 54  | m8    | 166  | LEU  | CB-CA-C    | -5.31 | 103.05      | 111.17   |
| 70  | o4    | 81   | CYS  | N-CA-C     | 5.31  | 116.81      | 109.54   |
| 17  | C5    | 55   | GLY  | N-CA-C     | -5.31 | 108.83      | 114.67   |
| 51  | M5    | 92   | LEU  | CA-C-N     | -5.31 | 113.41      | 122.11   |
| 51  | M5    | 92   | LEU  | C-N-CA     | -5.31 | 113.41      | 122.11   |
| 8   | s6    | 69   | LEU  | CA-C-N     | -5.31 | 113.21      | 119.84   |
| 8   | s6    | 69   | LEU  | C-N-CA     | -5.31 | 113.21      | 119.84   |
| 79  | Q3    | 57   | CYS  | N-CA-C     | 5.29  | 117.37      | 108.96   |
| 41  | l4    | 300  | ARG  | CA-C-N     | 5.29  | 126.45      | 119.84   |
| 41  | l4    | 300  | ARG  | C-N-CA     | 5.29  | 126.45      | 119.84   |
| 67  | o1    | 52   | ALA  | CA-C-N     | -5.28 | 113.47      | 119.28   |
| 67  | o1    | 52   | ALA  | C-N-CA     | -5.28 | 113.47      | 119.28   |
| 49  | m3    | 74   | GLY  | CA-C-N     | -5.28 | 112.78      | 121.92   |
| 49  | m3    | 74   | GLY  | C-N-CA     | -5.28 | 112.78      | 121.92   |
| 53  | m7    | 79   | THR  | N-CA-C     | -5.28 | 107.49      | 114.04   |
| 40  | l3    | 205  | VAL  | CB-CA-C    | -5.28 | 103.98      | 112.16   |
| 65  | n9    | 19   | ASN  | CA-C-N     | -5.28 | 118.54      | 122.18   |
| 65  | n9    | 19   | ASN  | C-N-CA     | -5.28 | 118.54      | 122.18   |
| 41  | L4    | 190  | GLY  | N-CA-C     | 5.28  | 125.68      | 113.18   |
| 56  | N0    | 51   | VAL  | CB-CA-C    | -5.27 | 103.97      | 111.40   |
| 1   | 6     | 1600 | A    | N9-C1'-C2' | 5.27  | 121.91      | 114.00   |
| 3   | s1    | 189  | ILE  | CA-C-N     | -5.27 | 115.45      | 120.83   |
| 3   | s1    | 189  | ILE  | C-N-CA     | -5.27 | 115.45      | 120.83   |
| 6   | s4    | 103  | TYR  | N-CA-C     | 5.27  | 117.49      | 110.53   |
| 61  | n5    | 43   | ALA  | O-C-N      | 5.27  | 125.65      | 121.17   |
| 24  | d2    | 74   | VAL  | CA-C-N     | -5.27 | 116.27      | 123.12   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | d2    | 74   | VAL  | C-N-CA      | -5.27 | 116.27      | 123.12   |
| 41  | L4    | 73   | ARG  | CB-CG-CD    | -5.26 | 99.19       | 111.30   |
| 54  | m8    | 54   | LEU  | N-CA-C      | 5.26  | 117.86      | 109.96   |
| 36  | 5     | 835  | G    | O4'-C1'-N9  | 5.26  | 116.09      | 108.20   |
| 40  | l3    | 310  | GLY  | CA-C-O      | -5.26 | 118.60      | 122.23   |
| 16  | C4    | 56   | SER  | CA-C-N      | 5.26  | 125.31      | 119.32   |
| 16  | C4    | 56   | SER  | C-N-CA      | 5.26  | 125.31      | 119.32   |
| 1   | 6     | 1568 | C    | C4'-C3'-O3' | 5.26  | 117.28      | 109.40   |
| 25  | d3    | 23   | ARG  | CG-CD-NE    | 5.25  | 123.56      | 112.00   |
| 42  | l5    | 118  | THR  | N-CA-C      | -5.25 | 102.50      | 110.28   |
| 49  | m3    | 58   | VAL  | CA-C-N      | -5.25 | 115.78      | 122.77   |
| 49  | m3    | 58   | VAL  | C-N-CA      | -5.25 | 115.78      | 122.77   |
| 41  | l4    | 190  | GLY  | N-CA-C      | 5.25  | 125.62      | 113.18   |
| 66  | o0    | 32   | LYS  | N-CA-C      | -5.24 | 105.57      | 111.28   |
| 42  | l5    | 43   | LYS  | N-CA-C      | -5.24 | 106.12      | 112.88   |
| 14  | C2    | 81   | ASP  | CA-C-N      | 5.23  | 126.38      | 119.84   |
| 14  | C2    | 81   | ASP  | C-N-CA      | 5.23  | 126.38      | 119.84   |
| 62  | n6    | 100  | HIS  | CA-C-N      | -5.23 | 114.43      | 119.87   |
| 62  | n6    | 100  | HIS  | C-N-CA      | -5.23 | 114.43      | 119.87   |
| 16  | c4    | 124  | ASP  | N-CA-C      | 5.23  | 121.94      | 110.80   |
| 27  | D5    | 95   | HIS  | N-CA-C      | 5.22  | 121.92      | 110.80   |
| 36  | 5     | 1481 | A    | P-O3'-C3'   | 5.22  | 128.03      | 120.20   |
| 31  | D9    | 14   | TYR  | N-CA-C      | 5.22  | 117.00      | 109.07   |
| 51  | M5    | 42   | PRO  | CA-C-O      | -5.22 | 115.51      | 121.56   |
| 2   | S0    | 105  | GLY  | N-CA-C      | -5.22 | 107.84      | 115.72   |
| 9   | S7    | 146  | GLY  | N-CA-C      | 5.22  | 122.30      | 115.47   |
| 4   | s2    | 237  | VAL  | N-CA-C      | 5.22  | 117.61      | 111.09   |
| 5   | s3    | 210  | GLU  | CA-C-N      | 5.22  | 125.95      | 120.11   |
| 5   | s3    | 210  | GLU  | C-N-CA      | 5.22  | 125.95      | 120.11   |
| 52  | m6    | 113  | ASP  | CA-C-N      | -5.21 | 114.80      | 122.83   |
| 52  | m6    | 113  | ASP  | C-N-CA      | -5.21 | 114.80      | 122.83   |
| 53  | M7    | 118  | GLN  | CA-C-N      | -5.21 | 116.31      | 123.14   |
| 53  | M7    | 118  | GLN  | C-N-CA      | -5.21 | 116.31      | 123.14   |
| 72  | o6    | 32   | ALA  | N-CA-C      | 5.21  | 117.64      | 110.35   |
| 52  | M6    | 175  | THR  | N-CA-C      | -5.20 | 106.88      | 113.18   |
| 73  | o7    | 58   | THR  | N-CA-C      | 5.20  | 116.81      | 110.41   |
| 66  | o0    | 9    | SER  | CB-CA-C     | -5.20 | 109.03      | 115.89   |
| 40  | L3    | 196  | ARG  | N-CA-C      | -5.20 | 105.70      | 111.36   |
| 68  | o2    | 40   | SER  | N-CA-C      | 5.20  | 118.00      | 110.42   |
| 39  | L2    | 47   | GLN  | CA-C-N      | -5.19 | 116.34      | 123.14   |
| 39  | L2    | 47   | GLN  | C-N-CA      | -5.19 | 116.34      | 123.14   |
| 45  | L8    | 186  | LEU  | N-CA-C      | -5.19 | 105.31      | 111.69   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | M5    | 183  | THR  | N-CA-C      | -5.18 | 98.57       | 107.23   |
| 40  | l3    | 330  | GLY  | CA-C-O      | -5.18 | 118.65      | 122.23   |
| 45  | l8    | 78   | PHE  | N-CA-C      | -5.18 | 103.69      | 110.53   |
| 36  | 1     | 2249 | G    | C2'-C3'-O3' | 5.18  | 121.47      | 113.70   |
| 44  | L7    | 227  | GLY  | N-CA-C      | -5.18 | 106.57      | 112.79   |
| 36  | 1     | 611  | A    | O5'-P-OP1   | 5.18  | 123.54      | 108.00   |
| 45  | L8    | 237  | ILE  | N-CA-C      | 5.18  | 115.55      | 107.99   |
| 22  | d0    | 71   | PRO  | N-CA-C      | -5.18 | 103.70      | 111.57   |
| 42  | l5    | 174  | PRO  | CA-C-O      | -5.18 | 115.68      | 121.32   |
| 9   | S7    | 55   | LYS  | N-CA-C      | 5.18  | 115.12      | 108.34   |
| 41  | L4    | 139  | GLY  | CA-C-O      | -5.18 | 114.26      | 122.28   |
| 66  | O0    | 79   | THR  | N-CA-C      | -5.17 | 105.71      | 112.23   |
| 51  | m5    | 183  | THR  | CB-CA-C     | -5.17 | 100.13      | 110.42   |
| 73  | O7    | 60   | GLY  | N-CA-C      | -5.17 | 107.87      | 114.85   |
| 52  | m6    | 83   | ALA  | N-CA-C      | -5.17 | 105.82      | 111.82   |
| 50  | M4    | 78   | THR  | N-CA-C      | 5.17  | 117.31      | 111.11   |
| 5   | S3    | 166  | ASP  | N-CA-C      | 5.17  | 116.72      | 111.14   |
| 41  | l4    | 269  | SER  | N-CA-C      | 5.16  | 118.68      | 112.38   |
| 43  | l6    | 66   | SER  | N-CA-C      | 5.16  | 121.80      | 110.80   |
| 47  | m0    | 10   | ARG  | N-CA-C      | 5.16  | 116.71      | 111.14   |
| 42  | L5    | 15   | ARG  | CA-C-N      | -5.15 | 114.13      | 121.50   |
| 42  | L5    | 15   | ARG  | C-N-CA      | -5.15 | 114.13      | 121.50   |
| 7   | S5    | 126  | ASP  | CB-CA-C     | -5.15 | 110.62      | 116.54   |
| 70  | O4    | 81   | CYS  | N-CA-C      | 5.15  | 119.66      | 113.17   |
| 36  | 1     | 99   | A    | C5'-C4'-O4' | 5.15  | 117.52      | 109.80   |
| 44  | L7    | 243  | MET  | N-CA-C      | -5.14 | 107.39      | 113.97   |
| 36  | 5     | 3016 | A    | OP1-P-O3'   | -5.14 | 92.57       | 108.00   |
| 36  | 5     | 2398 | A    | O5'-C5'-C4' | 5.14  | 119.21      | 111.50   |
| 61  | n5    | 107  | VAL  | N-CA-C      | 5.14  | 115.67      | 108.17   |
| 67  | o1    | 8    | VAL  | CB-CA-C     | -5.14 | 104.15      | 111.19   |
| 54  | m8    | 59   | ARG  | CA-C-N      | -5.13 | 115.09      | 120.38   |
| 54  | m8    | 59   | ARG  | C-N-CA      | -5.13 | 115.09      | 120.38   |
| 14  | C2    | 94   | ALA  | N-CA-C      | 5.13  | 116.88      | 111.28   |
| 28  | D6    | 97   | PRO  | N-CA-C      | 5.13  | 116.96      | 110.70   |
| 64  | N8    | 14   | HIS  | O-C-N       | -5.13 | 116.89      | 122.84   |
| 47  | m0    | 178  | ARG  | CA-C-N      | -5.13 | 113.26      | 118.85   |
| 47  | m0    | 178  | ARG  | C-N-CA      | -5.13 | 113.26      | 118.85   |
| 28  | D6    | 58   | VAL  | N-CA-C      | -5.13 | 104.46      | 110.05   |
| 79  | q3    | 16   | VAL  | N-CA-CB     | -5.13 | 106.57      | 112.21   |
| 19  | c7    | 106  | THR  | N-CA-C      | -5.12 | 105.82      | 111.71   |
| 46  | l9    | 7    | GLU  | N-CA-C      | 5.12  | 116.86      | 109.07   |
| 1   | 2     | 158  | U    | P-O3'-C3'   | 5.12  | 127.88      | 120.20   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 6     | 272  | U    | C2'-C3'-O3' | 5.12  | 117.18      | 109.50   |
| 36  | 1     | 65   | A    | P-O3'-C3'   | 5.12  | 127.88      | 120.20   |
| 44  | L7    | 119  | VAL  | CB-CA-C     | -5.12 | 105.70      | 111.23   |
| 58  | n2    | 62   | VAL  | N-CA-C      | 5.12  | 115.49      | 108.12   |
| 44  | l7    | 158  | LYS  | CB-CG-CD    | 5.10  | 123.03      | 111.30   |
| 22  | D0    | 62   | VAL  | N-CA-C      | 5.10  | 115.19      | 107.75   |
| 23  | D1    | 37   | ALA  | N-CA-C      | 5.10  | 117.09      | 109.59   |
| 49  | M3    | 76   | THR  | N-CA-CB     | 5.10  | 119.11      | 110.49   |
| 72  | O6    | 26   | ILE  | CB-CA-C     | -5.10 | 105.36      | 112.04   |
| 22  | d0    | 31   | VAL  | N-CA-C      | 5.10  | 116.43      | 110.62   |
| 64  | n8    | 65   | GLN  | CA-C-N      | -5.10 | 115.79      | 124.31   |
| 64  | n8    | 65   | GLN  | C-N-CA      | -5.10 | 115.79      | 124.31   |
| 74  | o8    | 55   | VAL  | N-CA-C      | 5.10  | 114.91      | 107.37   |
| 13  | C1    | 135  | VAL  | N-CA-C      | 5.09  | 116.08      | 108.54   |
| 53  | M7    | 169  | THR  | N-CA-C      | 5.09  | 116.50      | 110.19   |
| 40  | L3    | 264  | VAL  | N-CA-C      | 5.09  | 116.86      | 108.97   |
| 52  | M6    | 78   | ARG  | NE-CZ-NH1   | 5.09  | 126.59      | 121.50   |
| 52  | m6    | 94   | ARG  | NE-CZ-NH2   | 5.09  | 123.78      | 119.20   |
| 40  | l3    | 78   | VAL  | CA-C-N      | -5.08 | 116.88      | 123.19   |
| 40  | l3    | 78   | VAL  | C-N-CA      | -5.08 | 116.88      | 123.19   |
| 39  | L2    | 91   | GLY  | N-CA-C      | 5.08  | 117.01      | 110.96   |
| 41  | l4    | 330  | TYR  | CA-CB-CG    | -5.08 | 104.75      | 113.90   |
| 51  | M5    | 90   | ASN  | CA-C-N      | -5.08 | 114.19      | 123.34   |
| 51  | M5    | 90   | ASN  | C-N-CA      | -5.08 | 114.19      | 123.34   |
| 17  | C5    | 64   | LYS  | N-CA-C      | -5.07 | 107.22      | 113.41   |
| 16  | c4    | 132  | ARG  | N-CA-C      | 5.07  | 121.61      | 110.80   |
| 36  | 5     | 1308 | A    | C5'-C4'-C3' | -5.07 | 107.59      | 115.20   |
| 47  | M0    | 120  | GLY  | N-CA-C      | 5.06  | 120.26      | 112.51   |
| 4   | S2    | 170  | ILE  | CA-C-N      | 5.06  | 124.97      | 119.76   |
| 4   | S2    | 170  | ILE  | C-N-CA      | 5.06  | 124.97      | 119.76   |
| 15  | C3    | 59   | GLY  | N-CA-C      | -5.06 | 101.19      | 113.18   |
| 36  | 1     | 979  | U    | P-O3'-C3'   | 5.06  | 127.78      | 120.20   |
| 16  | c4    | 136  | ARG  | N-CA-C      | 5.06  | 116.66      | 108.41   |
| 47  | m0    | 20   | SER  | N-CA-C      | 5.06  | 115.01      | 107.88   |
| 4   | s2    | 186  | LYS  | N-CA-C      | -5.06 | 105.66      | 111.07   |
| 13  | c1    | 61   | THR  | N-CA-C      | 5.06  | 121.57      | 110.80   |
| 25  | d3    | 95   | PHE  | CA-C-N      | -5.05 | 116.09      | 123.06   |
| 25  | d3    | 95   | PHE  | C-N-CA      | -5.05 | 116.09      | 123.06   |
| 44  | l7    | 213  | GLY  | N-CA-C      | 5.05  | 121.42      | 112.83   |
| 40  | L3    | 318  | LYS  | N-CA-C      | -5.05 | 105.49      | 113.02   |
| 1   | 6     | 1196 | A    | C4'-C3'-O3' | 5.05  | 116.98      | 109.40   |
| 49  | m3    | 76   | THR  | N-CA-CB     | 5.05  | 119.03      | 110.49   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 64  | n8    | 128  | ARG  | N-CA-C    | -5.05 | 102.22      | 110.20   |
| 64  | N8    | 46   | ASP  | CA-C-O    | -5.05 | 116.20      | 121.55   |
| 40  | L3    | 72   | VAL  | CA-C-N    | -5.05 | 116.59      | 123.10   |
| 40  | L3    | 72   | VAL  | C-N-CA    | -5.05 | 116.59      | 123.10   |
| 46  | l9    | 82   | VAL  | N-CA-C    | -5.05 | 108.06      | 112.90   |
| 21  | C9    | 9    | VAL  | N-CA-C    | 5.04  | 115.38      | 108.12   |
| 53  | M7    | 183  | ALA  | CB-CA-C   | -5.04 | 109.81      | 117.07   |
| 4   | S2    | 226  | THR  | CA-C-N    | -5.04 | 114.47      | 119.56   |
| 4   | S2    | 226  | THR  | C-N-CA    | -5.04 | 114.47      | 119.56   |
| 7   | S5    | 141  | GLY  | CA-C-N    | 5.04  | 126.14      | 119.84   |
| 7   | S5    | 141  | GLY  | C-N-CA    | 5.04  | 126.14      | 119.84   |
| 43  | l6    | 173  | MET  | CB-CG-SD  | -5.04 | 97.59       | 112.70   |
| 6   | S4    | 229  | GLY  | N-CA-C    | 5.03  | 116.84      | 110.20   |
| 43  | L6    | 102  | ASN  | N-CA-C    | 5.03  | 115.01      | 108.07   |
| 3   | s1    | 145  | LYS  | CA-C-N    | -5.03 | 114.31      | 122.36   |
| 3   | s1    | 145  | LYS  | C-N-CA    | -5.03 | 114.31      | 122.36   |
| 57  | n1    | 17   | ARG  | CA-CB-CG  | -5.03 | 104.04      | 114.10   |
| 40  | l3    | 277  | SER  | CA-C-N    | -5.03 | 116.89      | 122.27   |
| 40  | l3    | 277  | SER  | C-N-CA    | -5.03 | 116.89      | 122.27   |
| 41  | l4    | 23   | PRO  | CA-C-O    | -5.03 | 111.45      | 120.60   |
| 47  | M0    | 115  | MET  | N-CA-C    | -5.03 | 106.57      | 113.30   |
| 51  | M5    | 85   | THR  | CB-CA-C   | -5.03 | 98.92       | 110.18   |
| 53  | M7    | 59   | PRO  | CA-C-O    | -5.03 | 115.30      | 121.03   |
| 5   | s3    | 167  | PHE  | CA-C-N    | -5.03 | 116.62      | 123.10   |
| 5   | s3    | 167  | PHE  | C-N-CA    | -5.03 | 116.62      | 123.10   |
| 5   | s3    | 4    | LEU  | N-CA-C    | 5.02  | 118.17      | 111.24   |
| 4   | S2    | 150  | GLN  | CA-C-N    | 5.02  | 125.02      | 119.90   |
| 4   | S2    | 150  | GLN  | C-N-CA    | 5.02  | 125.02      | 119.90   |
| 36  | 1     | 2373 | A    | O5'-P-OP1 | -5.02 | 92.94       | 108.00   |
| 52  | m6    | 166  | GLU  | N-CA-C    | -5.02 | 105.89      | 111.36   |
| 34  | SR    | 126  | SER  | N-CA-C    | 5.02  | 116.47      | 108.79   |
| 36  | 1     | 1381 | A    | O5'-P-OP2 | 5.02  | 123.06      | 108.00   |
| 39  | l2    | 216  | HIS  | CA-C-O    | -5.02 | 115.24      | 121.06   |
| 13  | c1    | 60   | PHE  | N-CA-C    | -5.02 | 102.64      | 110.42   |
| 18  | c6    | 48   | VAL  | N-CA-C    | -5.02 | 107.55      | 113.42   |
| 46  | L9    | 16   | VAL  | N-CA-C    | 5.01  | 117.03      | 108.86   |
| 46  | L9    | 134  | ILE  | N-CA-C    | 5.01  | 115.33      | 108.12   |
| 2   | S0    | 202  | TYR  | N-CA-C    | -5.01 | 102.97      | 110.23   |
| 26  | d4    | 60   | PHE  | N-CA-C    | 5.01  | 116.92      | 108.96   |
| 40  | L3    | 174  | LYS  | N-CA-C    | 5.00  | 121.46      | 110.80   |

There are no chirality outliers.

All (57) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 16  | C4    | 123 | SER  | Peptide   |
| 16  | C4    | 124 | ASP  | Peptide   |
| 19  | C7    | 22  | PRO  | Peptide   |
| 25  | D3    | 3   | LYS  | Peptide   |
| 27  | D5    | 94  | LYS  | Peptide   |
| 28  | D6    | 84  | VAL  | Peptide   |
| 28  | D6    | 85  | ARG  | Peptide   |
| 28  | D6    | 97  | PRO  | Peptide   |
| 33  | E1    | 137 | ASP  | Peptide   |
| 39  | L2    | 19  | HIS  | Peptide   |
| 41  | L4    | 190 | GLY  | Peptide   |
| 41  | L4    | 318 | LEU  | Peptide   |
| 42  | L5    | 257 | GLU  | Peptide   |
| 44  | L7    | 157 | ASN  | Peptide   |
| 51  | M5    | 182 | ASN  | Peptide   |
| 52  | M6    | 110 | PRO  | Peptide   |
| 52  | M6    | 111 | PRO  | Peptide   |
| 53  | M7    | 8   | SER  | Peptide   |
| 57  | N1    | 16  | GLN  | Peptide   |
| 63  | N7    | 3   | LYS  | Peptide   |
| 65  | N9    | 19  | ASN  | Peptide   |
| 67  | O1    | 5   | LYS  | Peptide   |
| 72  | O6    | 2   | THR  | Peptide   |
| 2   | S0    | 188 | LEU  | Peptide   |
| 9   | S7    | 131 | PHE  | Peptide   |
| 10  | S8    | 147 | ALA  | Peptide   |
| 34  | SR    | 160 | GLU  | Mainchain |
| 34  | SR    | 161 | LYS  | Mainchain |
| 17  | c5    | 52  | LYS  | Peptide   |
| 22  | d0    | 70  | THR  | Peptide   |
| 25  | d3    | 44  | GLY  | Peptide   |
| 26  | d4    | 29  | HIS  | Peptide   |
| 26  | d4    | 50  | ALA  | Peptide   |
| 31  | d9    | 17  | GLY  | Peptide   |
| 39  | l2    | 143 | GLU  | Peptide   |
| 39  | l2    | 171 | GLY  | Peptide   |
| 40  | l3    | 139 | GLN  | Peptide   |
| 40  | l3    | 185 | GLY  | Peptide   |
| 41  | l4    | 91  | GLY  | Peptide   |
| 42  | l5    | 270 | LYS  | Peptide   |
| 42  | l5    | 271 | LYS  | Peptide   |
| 43  | l6    | 51  | ARG  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 44  | l7    | 192 | GLY  | Peptide |
| 44  | l7    | 226 | GLY  | Peptide |
| 52  | m6    | 110 | PRO  | Peptide |
| 53  | m7    | 66  | SER  | Peptide |
| 59  | n3    | 41  | GLY  | Peptide |
| 62  | n6    | 111 | LEU  | Peptide |
| 63  | n7    | 6   | LYS  | Peptide |
| 64  | n8    | 66  | ALA  | Peptide |
| 64  | n8    | 75  | LEU  | Peptide |
| 65  | n9    | 19  | ASN  | Peptide |
| 65  | n9    | 23  | LYS  | Peptide |
| 65  | n9    | 24  | PRO  | Peptide |
| 67  | o1    | 64  | VAL  | Peptide |
| 7   | s5    | 44  | ASN  | Peptide |
| 7   | s5    | 99  | MET  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 37283 | 0        | 18757    | 752     | 0            |
| 1   | 6     | 38238 | 0        | 19241    | 718     | 0            |
| 2   | S0    | 1577  | 0        | 1567     | 83      | 0            |
| 2   | s0    | 1583  | 0        | 1578     | 74      | 0            |
| 3   | S1    | 1709  | 0        | 1784     | 89      | 0            |
| 3   | s1    | 1722  | 0        | 1793     | 67      | 0            |
| 4   | S2    | 1635  | 0        | 1723     | 64      | 0            |
| 4   | s2    | 1635  | 0        | 1723     | 60      | 0            |
| 5   | S3    | 1734  | 0        | 1817     | 54      | 0            |
| 5   | s3    | 1734  | 0        | 1817     | 50      | 0            |
| 6   | S4    | 2068  | 0        | 2154     | 72      | 0            |
| 6   | s4    | 2068  | 0        | 2154     | 92      | 0            |
| 7   | S5    | 1609  | 0        | 1675     | 65      | 0            |
| 7   | s5    | 1609  | 0        | 1675     | 78      | 0            |
| 8   | S6    | 1799  | 0        | 1879     | 62      | 0            |
| 8   | s6    | 1755  | 0        | 1846     | 55      | 0            |
| 9   | S7    | 1481  | 0        | 1572     | 62      | 0            |
| 9   | s7    | 1491  | 0        | 1578     | 47      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | S8    | 1489  | 0        | 1525     | 56      | 0            |
| 10  | s8    | 1489  | 0        | 1525     | 50      | 0            |
| 11  | S9    | 1494  | 0        | 1573     | 63      | 0            |
| 11  | s9    | 1494  | 0        | 1573     | 62      | 0            |
| 12  | C0    | 773   | 0        | 729      | 37      | 0            |
| 12  | c0    | 762   | 0        | 699      | 27      | 0            |
| 13  | C1    | 1214  | 0        | 1259     | 29      | 0            |
| 13  | c1    | 1168  | 0        | 1231     | 35      | 0            |
| 14  | C2    | 890   | 0        | 887      | 37      | 0            |
| 14  | c2    | 890   | 0        | 887      | 32      | 0            |
| 15  | C3    | 1192  | 0        | 1255     | 46      | 0            |
| 15  | c3    | 1192  | 0        | 1255     | 37      | 0            |
| 16  | C4    | 891   | 0        | 883      | 53      | 0            |
| 16  | c4    | 949   | 0        | 985      | 49      | 0            |
| 17  | C5    | 977   | 0        | 1002     | 34      | 0            |
| 17  | c5    | 1039  | 0        | 1050     | 46      | 0            |
| 18  | C6    | 1105  | 0        | 1166     | 51      | 0            |
| 18  | c6    | 1111  | 0        | 1171     | 45      | 0            |
| 19  | C7    | 926   | 0        | 930      | 40      | 0            |
| 19  | c7    | 906   | 0        | 909      | 41      | 0            |
| 20  | C8    | 1192  | 0        | 1222     | 41      | 0            |
| 20  | c8    | 1192  | 0        | 1222     | 57      | 0            |
| 21  | C9    | 1112  | 0        | 1124     | 56      | 0            |
| 21  | c9    | 1112  | 0        | 1124     | 35      | 0            |
| 22  | D0    | 855   | 0        | 917      | 47      | 0            |
| 22  | d0    | 882   | 0        | 939      | 36      | 0            |
| 23  | D1    | 684   | 0        | 672      | 33      | 0            |
| 23  | d1    | 684   | 0        | 672      | 26      | 0            |
| 24  | D2    | 1021  | 0        | 1060     | 39      | 0            |
| 24  | d2    | 1021  | 0        | 1060     | 33      | 0            |
| 25  | D3    | 1121  | 0        | 1196     | 43      | 0            |
| 25  | d3    | 1121  | 0        | 1196     | 37      | 0            |
| 26  | D4    | 1073  | 0        | 1132     | 45      | 0            |
| 26  | d4    | 1073  | 0        | 1132     | 28      | 0            |
| 27  | D5    | 563   | 0        | 603      | 29      | 0            |
| 27  | d5    | 558   | 0        | 598      | 25      | 0            |
| 28  | D6    | 769   | 0        | 814      | 50      | 0            |
| 28  | d6    | 769   | 0        | 814      | 36      | 0            |
| 29  | D7    | 610   | 0        | 631      | 24      | 0            |
| 29  | d7    | 610   | 0        | 631      | 28      | 0            |
| 30  | D8    | 497   | 0        | 535      | 17      | 0            |
| 30  | d8    | 497   | 0        | 535      | 20      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | D9    | 442   | 0        | 428      | 19      | 0            |
| 31  | d9    | 442   | 0        | 428      | 18      | 0            |
| 32  | E0    | 475   | 0        | 525      | 8       | 0            |
| 33  | E1    | 566   | 0        | 602      | 39      | 0            |
| 33  | e1    | 608   | 0        | 657      | 32      | 0            |
| 34  | SR    | 2441  | 0        | 2395     | 74      | 0            |
| 34  | sR    | 2442  | 0        | 2392     | 70      | 0            |
| 35  | SM    | 1104  | 0        | 996      | 38      | 0            |
| 35  | sM    | 680   | 0        | 607      | 33      | 0            |
| 36  | 1     | 67355 | 0        | 33840    | 1048    | 0            |
| 36  | 5     | 67376 | 0        | 33857    | 1050    | 0            |
| 37  | 3     | 2579  | 0        | 1304     | 39      | 0            |
| 37  | 7     | 2579  | 0        | 1304     | 42      | 0            |
| 38  | 4     | 3353  | 0        | 1695     | 51      | 0            |
| 38  | 8     | 3353  | 0        | 1695     | 59      | 0            |
| 39  | L2    | 1914  | 0        | 1981     | 55      | 0            |
| 39  | l2    | 1912  | 0        | 1976     | 88      | 0            |
| 40  | L3    | 3075  | 0        | 3142     | 148     | 0            |
| 40  | l3    | 3075  | 0        | 3142     | 114     | 0            |
| 41  | L4    | 2748  | 0        | 2859     | 100     | 0            |
| 41  | l4    | 2748  | 0        | 2859     | 105     | 0            |
| 42  | L5    | 2375  | 0        | 2325     | 97      | 0            |
| 42  | l5    | 2359  | 0        | 2311     | 89      | 0            |
| 43  | L6    | 1239  | 0        | 1326     | 29      | 0            |
| 43  | l6    | 1248  | 0        | 1339     | 44      | 0            |
| 44  | L7    | 1784  | 0        | 1862     | 45      | 0            |
| 44  | l7    | 1791  | 0        | 1869     | 41      | 0            |
| 45  | L8    | 1804  | 0        | 1877     | 66      | 0            |
| 45  | l8    | 1763  | 0        | 1819     | 60      | 0            |
| 46  | L9    | 1518  | 0        | 1587     | 71      | 0            |
| 46  | l9    | 1518  | 0        | 1587     | 49      | 0            |
| 47  | M0    | 1705  | 0        | 1736     | 63      | 0            |
| 47  | m0    | 1722  | 0        | 1755     | 59      | 0            |
| 48  | M1    | 1353  | 0        | 1383     | 51      | 0            |
| 48  | m1    | 1353  | 0        | 1383     | 48      | 0            |
| 49  | M3    | 1543  | 0        | 1608     | 52      | 0            |
| 49  | m3    | 1548  | 0        | 1613     | 48      | 0            |
| 50  | M4    | 1053  | 0        | 1149     | 32      | 0            |
| 50  | m4    | 1059  | 0        | 1154     | 30      | 0            |
| 51  | M5    | 1720  | 0        | 1779     | 66      | 0            |
| 51  | m5    | 1720  | 0        | 1779     | 66      | 0            |
| 52  | M6    | 1555  | 0        | 1659     | 42      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52  | m6    | 1555  | 0        | 1659     | 50      | 0            |
| 53  | M7    | 1420  | 0        | 1437     | 49      | 0            |
| 53  | m7    | 1227  | 0        | 1236     | 43      | 0            |
| 54  | M8    | 1441  | 0        | 1543     | 48      | 0            |
| 54  | m8    | 1441  | 0        | 1543     | 48      | 0            |
| 55  | M9    | 1521  | 0        | 1617     | 48      | 0            |
| 55  | m9    | 1521  | 0        | 1617     | 30      | 0            |
| 56  | N0    | 1445  | 0        | 1487     | 43      | 0            |
| 56  | n0    | 1445  | 0        | 1487     | 41      | 0            |
| 57  | N1    | 1276  | 0        | 1323     | 44      | 0            |
| 57  | n1    | 1276  | 0        | 1323     | 46      | 0            |
| 58  | N2    | 796   | 0        | 812      | 14      | 0            |
| 58  | n2    | 778   | 0        | 791      | 17      | 0            |
| 59  | N3    | 1003  | 0        | 1048     | 49      | 0            |
| 59  | n3    | 1003  | 0        | 1048     | 29      | 0            |
| 60  | N4    | 699   | 0        | 640      | 17      | 0            |
| 60  | n4    | 1038  | 0        | 1071     | 18      | 0            |
| 61  | N5    | 964   | 0        | 1025     | 41      | 0            |
| 61  | n5    | 959   | 0        | 1023     | 31      | 0            |
| 62  | N6    | 993   | 0        | 1081     | 24      | 0            |
| 62  | n6    | 993   | 0        | 1081     | 37      | 0            |
| 63  | N7    | 1092  | 0        | 1155     | 47      | 0            |
| 63  | n7    | 1092  | 0        | 1155     | 39      | 0            |
| 64  | N8    | 1173  | 0        | 1215     | 54      | 0            |
| 64  | n8    | 1173  | 0        | 1215     | 53      | 0            |
| 65  | N9    | 462   | 0        | 491      | 14      | 0            |
| 65  | n9    | 462   | 0        | 491      | 21      | 0            |
| 66  | O0    | 743   | 0        | 797      | 27      | 0            |
| 66  | o0    | 767   | 0        | 816      | 28      | 0            |
| 67  | O1    | 876   | 0        | 912      | 25      | 0            |
| 67  | o1    | 883   | 0        | 918      | 21      | 0            |
| 68  | O2    | 1020  | 0        | 1090     | 17      | 0            |
| 68  | o2    | 1020  | 0        | 1090     | 38      | 0            |
| 69  | O3    | 850   | 0        | 880      | 28      | 0            |
| 69  | o3    | 850   | 0        | 880      | 28      | 0            |
| 70  | O4    | 880   | 0        | 945      | 25      | 0            |
| 70  | o4    | 880   | 0        | 945      | 35      | 0            |
| 71  | O5    | 969   | 0        | 1078     | 31      | 0            |
| 71  | o5    | 965   | 0        | 1067     | 37      | 0            |
| 72  | O6    | 771   | 0        | 849      | 32      | 0            |
| 72  | o6    | 770   | 0        | 846      | 29      | 0            |
| 73  | O7    | 681   | 0        | 683      | 33      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 73  | o7    | 681   | 0        | 683      | 31      | 0            |
| 74  | O8    | 612   | 0        | 682      | 23      | 0            |
| 74  | o8    | 608   | 0        | 671      | 27      | 0            |
| 75  | O9    | 436   | 0        | 475      | 18      | 0            |
| 75  | o9    | 436   | 0        | 475      | 19      | 0            |
| 76  | Q0    | 417   | 0        | 455      | 14      | 0            |
| 76  | q0    | 417   | 0        | 455      | 13      | 0            |
| 77  | Q1    | 233   | 0        | 284      | 15      | 0            |
| 77  | q1    | 233   | 0        | 284      | 13      | 0            |
| 78  | Q2    | 847   | 0        | 916      | 35      | 0            |
| 78  | q2    | 847   | 0        | 914      | 20      | 0            |
| 79  | Q3    | 694   | 0        | 734      | 22      | 0            |
| 79  | q3    | 694   | 0        | 734      | 26      | 0            |
| 80  | e0    | 491   | 0        | 542      | 19      | 0            |
| 81  | m2    | 750   | 0        | 175      | 13      | 0            |
| 82  | p0    | 1077  | 0        | 1041     | 39      | 0            |
| 83  | p1    | 235   | 0        | 51       | 4       | 0            |
| 84  | p2    | 230   | 0        | 50       | 1       | 0            |
| 85  | 1     | 475   | 0        | 0        | 0       | 0            |
| 85  | 2     | 126   | 0        | 0        | 0       | 0            |
| 85  | 3     | 14    | 0        | 0        | 0       | 0            |
| 85  | 4     | 21    | 0        | 0        | 0       | 0            |
| 85  | 5     | 504   | 0        | 0        | 0       | 0            |
| 85  | 6     | 147   | 0        | 0        | 0       | 0            |
| 85  | 7     | 15    | 0        | 0        | 0       | 0            |
| 85  | 8     | 13    | 0        | 0        | 0       | 0            |
| 85  | C3    | 1     | 0        | 0        | 0       | 0            |
| 85  | L2    | 1     | 0        | 0        | 0       | 0            |
| 85  | L3    | 2     | 0        | 0        | 0       | 0            |
| 85  | L4    | 3     | 0        | 0        | 0       | 0            |
| 85  | L5    | 1     | 0        | 0        | 0       | 0            |
| 85  | L6    | 1     | 0        | 0        | 0       | 0            |
| 85  | L7    | 2     | 0        | 0        | 0       | 0            |
| 85  | L8    | 1     | 0        | 0        | 0       | 0            |
| 85  | M0    | 2     | 0        | 0        | 0       | 0            |
| 85  | M1    | 1     | 0        | 0        | 0       | 0            |
| 85  | M3    | 4     | 0        | 0        | 0       | 0            |
| 85  | M5    | 2     | 0        | 0        | 0       | 0            |
| 85  | M6    | 1     | 0        | 0        | 0       | 0            |
| 85  | M7    | 6     | 0        | 0        | 0       | 0            |
| 85  | M9    | 1     | 0        | 0        | 0       | 0            |
| 85  | N0    | 1     | 0        | 0        | 0       | 0            |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 85  | N3    | 3     | 0        | 0        | 0       | 0            |
| 85  | N5    | 1     | 0        | 0        | 0       | 0            |
| 85  | N8    | 2     | 0        | 0        | 0       | 0            |
| 85  | O3    | 1     | 0        | 0        | 0       | 0            |
| 85  | O4    | 1     | 0        | 0        | 0       | 0            |
| 85  | O7    | 1     | 0        | 0        | 0       | 0            |
| 85  | Q2    | 1     | 0        | 0        | 0       | 0            |
| 85  | S8    | 1     | 0        | 0        | 0       | 0            |
| 85  | SM    | 1     | 0        | 0        | 0       | 0            |
| 85  | c1    | 1     | 0        | 0        | 0       | 0            |
| 85  | c7    | 1     | 0        | 0        | 0       | 0            |
| 85  | c8    | 2     | 0        | 0        | 0       | 0            |
| 85  | d2    | 1     | 0        | 0        | 0       | 0            |
| 85  | d3    | 1     | 0        | 0        | 0       | 0            |
| 85  | d6    | 1     | 0        | 0        | 0       | 0            |
| 85  | l2    | 2     | 0        | 0        | 0       | 0            |
| 85  | l3    | 1     | 0        | 0        | 0       | 0            |
| 85  | l4    | 1     | 0        | 0        | 0       | 0            |
| 85  | l5    | 3     | 0        | 0        | 0       | 0            |
| 85  | l7    | 1     | 0        | 0        | 0       | 0            |
| 85  | m1    | 2     | 0        | 0        | 0       | 0            |
| 85  | m4    | 1     | 0        | 0        | 0       | 0            |
| 85  | m5    | 1     | 0        | 0        | 0       | 0            |
| 85  | m6    | 1     | 0        | 0        | 0       | 0            |
| 85  | m7    | 5     | 0        | 0        | 0       | 0            |
| 85  | n0    | 2     | 0        | 0        | 0       | 0            |
| 85  | n3    | 2     | 0        | 0        | 0       | 0            |
| 85  | n6    | 2     | 0        | 0        | 0       | 0            |
| 85  | n8    | 4     | 0        | 0        | 0       | 0            |
| 85  | n9    | 2     | 0        | 0        | 0       | 0            |
| 85  | o1    | 1     | 0        | 0        | 0       | 0            |
| 85  | o3    | 2     | 0        | 0        | 0       | 0            |
| 85  | o4    | 2     | 0        | 0        | 0       | 0            |
| 85  | q0    | 1     | 0        | 0        | 0       | 0            |
| 85  | q1    | 1     | 0        | 0        | 0       | 0            |
| 85  | q3    | 1     | 0        | 0        | 0       | 0            |
| 85  | s1    | 1     | 0        | 0        | 0       | 0            |
| 85  | s6    | 1     | 0        | 0        | 0       | 0            |
| 85  | s8    | 2     | 0        | 0        | 0       | 0            |
| 85  | sM    | 2     | 0        | 0        | 0       | 0            |
| 86  | 1     | 2436  | 0        | 0        | 247     | 0            |
| 86  | 2     | 1106  | 0        | 0        | 132     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86  | 3     | 84    | 0        | 0        | 5       | 0            |
| 86  | 4     | 105   | 0        | 0        | 5       | 0            |
| 86  | 5     | 2471  | 0        | 0        | 236     | 0            |
| 86  | 6     | 1106  | 0        | 0        | 101     | 0            |
| 86  | 7     | 84    | 0        | 0        | 12      | 0            |
| 86  | 8     | 112   | 0        | 0        | 21      | 0            |
| 86  | C1    | 7     | 0        | 0        | 7       | 0            |
| 86  | C3    | 7     | 0        | 0        | 1       | 0            |
| 86  | C5    | 7     | 0        | 0        | 2       | 0            |
| 86  | C8    | 7     | 0        | 0        | 1       | 0            |
| 86  | D9    | 7     | 0        | 0        | 0       | 0            |
| 86  | L3    | 14    | 0        | 0        | 1       | 0            |
| 86  | L4    | 7     | 0        | 0        | 2       | 0            |
| 86  | L6    | 7     | 0        | 0        | 0       | 0            |
| 86  | M0    | 7     | 0        | 0        | 0       | 0            |
| 86  | M5    | 14    | 0        | 0        | 2       | 0            |
| 86  | M6    | 7     | 0        | 0        | 1       | 0            |
| 86  | M7    | 14    | 0        | 0        | 1       | 0            |
| 86  | M9    | 7     | 0        | 0        | 1       | 0            |
| 86  | N9    | 7     | 0        | 0        | 1       | 0            |
| 86  | O2    | 7     | 0        | 0        | 0       | 0            |
| 86  | O3    | 7     | 0        | 0        | 0       | 0            |
| 86  | O7    | 14    | 0        | 0        | 7       | 0            |
| 86  | O9    | 7     | 0        | 0        | 4       | 0            |
| 86  | Q2    | 7     | 0        | 0        | 2       | 0            |
| 86  | S8    | 7     | 0        | 0        | 1       | 0            |
| 86  | SR    | 7     | 0        | 0        | 0       | 0            |
| 86  | c1    | 7     | 0        | 0        | 7       | 0            |
| 86  | c3    | 7     | 0        | 0        | 3       | 0            |
| 86  | c5    | 7     | 0        | 0        | 2       | 0            |
| 86  | c8    | 7     | 0        | 0        | 0       | 0            |
| 86  | d4    | 7     | 0        | 0        | 0       | 0            |
| 86  | d9    | 7     | 0        | 0        | 1       | 0            |
| 86  | l3    | 21    | 0        | 0        | 0       | 0            |
| 86  | l4    | 14    | 0        | 0        | 3       | 0            |
| 86  | l5    | 21    | 0        | 0        | 1       | 0            |
| 86  | l9    | 7     | 0        | 0        | 0       | 0            |
| 86  | m0    | 14    | 0        | 0        | 2       | 0            |
| 86  | m1    | 7     | 0        | 0        | 1       | 0            |
| 86  | m4    | 7     | 0        | 0        | 0       | 0            |
| 86  | m5    | 7     | 0        | 0        | 0       | 0            |
| 86  | m6    | 7     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 86  | m7    | 7      | 0        | 0        | 1       | 0            |
| 86  | m8    | 7      | 0        | 0        | 0       | 0            |
| 86  | n3    | 7      | 0        | 0        | 0       | 0            |
| 86  | n9    | 7      | 0        | 0        | 0       | 0            |
| 86  | o2    | 7      | 0        | 0        | 0       | 0            |
| 86  | o3    | 7      | 0        | 0        | 0       | 0            |
| 86  | o4    | 7      | 0        | 0        | 4       | 0            |
| 86  | o7    | 7      | 0        | 0        | 1       | 0            |
| 86  | q2    | 7      | 0        | 0        | 3       | 0            |
| 86  | s1    | 14     | 0        | 0        | 1       | 0            |
| 86  | s4    | 7      | 0        | 0        | 1       | 0            |
| 86  | s8    | 7      | 0        | 0        | 1       | 0            |
| 86  | s9    | 7      | 0        | 0        | 2       | 0            |
| 86  | sR    | 7      | 0        | 0        | 0       | 0            |
| 87  | D6    | 1      | 0        | 0        | 0       | 0            |
| 87  | D7    | 1      | 0        | 0        | 0       | 0            |
| 87  | D9    | 1      | 0        | 0        | 0       | 0            |
| 87  | E1    | 1      | 0        | 0        | 0       | 0            |
| 87  | O7    | 1      | 0        | 0        | 0       | 0            |
| 87  | Q0    | 1      | 0        | 0        | 0       | 0            |
| 87  | Q2    | 1      | 0        | 0        | 3       | 0            |
| 87  | Q3    | 1      | 0        | 0        | 0       | 0            |
| 87  | d6    | 1      | 0        | 0        | 0       | 0            |
| 87  | d7    | 1      | 0        | 0        | 0       | 0            |
| 87  | d9    | 1      | 0        | 0        | 0       | 0            |
| 87  | e1    | 1      | 0        | 0        | 0       | 0            |
| 87  | o7    | 1      | 0        | 0        | 0       | 0            |
| 87  | q0    | 1      | 0        | 0        | 0       | 0            |
| 87  | q2    | 1      | 0        | 0        | 0       | 0            |
| 87  | q3    | 1      | 0        | 0        | 0       | 0            |
| 88  | 1     | 33     | 0        | 35       | 1       | 0            |
| 88  | 5     | 33     | 0        | 35       | 1       | 0            |
| All | All   | 411226 | 0        | 297341   | 9121    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (9121) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 52:m6:66:LYS:NZ | 52:m6:66:LYS:CE | 1.70                     | 1.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 78:Q2:17:CYS:SG    | 78:Q2:17:CYS:CB   | 2.09                     | 1.40              |
| 78:Q2:17:CYS:CB    | 87:Q2:501:ZN:ZN   | 1.31                     | 1.09              |
| 40:l3:296:THR:HG22 | 40:l3:298:PHE:H   | 1.18                     | 1.07              |
| 47:m0:76:MET:HE1   | 47:m0:148:VAL:HA  | 1.34                     | 1.05              |
| 36:5:2403:G:N2     | 36:5:2404:A:N7    | 2.03                     | 1.03              |
| 36:1:979:U:H1'     | 36:1:980:A:C8     | 1.94                     | 1.03              |
| 36:5:1639:C:OP2    | 70:o4:74:ARG:NH2  | 1.93                     | 1.01              |
| 4:S2:140:ARG:NH1   | 23:D1:1:MET:SD    | 2.34                     | 1.00              |
| 36:5:640:U:OP1     | 64:n8:21:ARG:NH2  | 1.96                     | 0.99              |
| 47:M0:174:THR:HG23 | 47:M0:176:LEU:H   | 1.25                     | 0.98              |
| 36:5:3274:A:H3'    | 36:5:3275:U:H5''  | 1.44                     | 0.98              |
| 50:m4:113:THR:HG22 | 50:m4:116:GLU:H   | 1.28                     | 0.97              |
| 10:S8:76:THR:HG22  | 10:S8:108:PRO:HG2 | 1.47                     | 0.97              |
| 69:O3:48:ARG:HG2   | 69:O3:48:ARG:HH11 | 1.28                     | 0.97              |
| 1:6:1011:G:OP2     | 86:6:2121:OHX:N3  | 1.97                     | 0.96              |
| 36:5:31:C:OP2      | 51:m5:188:ARG:NH2 | 1.98                     | 0.96              |
| 1:6:448:C:OP2      | 6:s4:49:ARG:NH1   | 1.98                     | 0.95              |
| 1:2:1585:U:H3      | 1:2:1611:A:H2     | 1.10                     | 0.95              |
| 36:1:640:U:OP1     | 64:N8:21:ARG:NH2  | 2.00                     | 0.95              |
| 49:m3:46:ILE:HG22  | 49:m3:49:ARG:HB2  | 1.48                     | 0.95              |
| 36:1:3346:U:H3     | 36:1:3359:A:H61   | 1.09                     | 0.94              |
| 1:2:1339:C:O2'     | 1:2:1341:A:N7     | 1.99                     | 0.94              |
| 36:5:3214:U:OP2    | 50:m4:128:ARG:NH2 | 2.00                     | 0.94              |
| 36:5:2853:A:H5'    | 47:m0:63:GLU:HB2  | 1.50                     | 0.94              |
| 41:l4:99:MET:HE3   | 41:l4:102:PRO:HA  | 1.49                     | 0.94              |
| 1:2:1588:G:H1      | 1:2:1608:U:H3     | 1.16                     | 0.93              |
| 36:1:31:C:OP2      | 51:M5:188:ARG:NH2 | 2.00                     | 0.93              |
| 36:1:2403:G:N2     | 36:1:2404:A:N7    | 2.15                     | 0.93              |
| 86:6:2159:OHX:N2   | 25:d3:64:PRO:O    | 2.02                     | 0.93              |
| 36:1:3343:G:H21    | 36:1:3362:A:H2    | 1.09                     | 0.92              |
| 78:q2:17:CYS:SG    | 78:q2:77:CYS:HB3  | 2.08                     | 0.92              |
| 86:5:4002:OHX:N3   | 44:l7:217:PRO:O   | 2.03                     | 0.92              |
| 36:5:3343:G:H21    | 36:5:3362:A:H2    | 1.10                     | 0.92              |
| 39:l2:204:MET:HE2  | 39:l2:209:HIS:HB2 | 1.49                     | 0.91              |
| 36:5:2273:G:O6     | 86:5:4196:OHX:N5  | 2.04                     | 0.90              |
| 36:1:1481:A:O2'    | 36:1:1858:A:N3    | 2.05                     | 0.90              |
| 1:6:383:G:N7       | 86:6:2149:OHX:N5  | 2.18                     | 0.90              |
| 20:c8:41:ARG:NH2   | 21:c9:36:ILE:O    | 2.04                     | 0.90              |
| 16:c4:50:ALA:O     | 16:c4:52:ARG:N    | 2.04                     | 0.90              |
| 40:l3:41:VAL:HA    | 40:l3:185:GLY:HA3 | 1.53                     | 0.90              |
| 50:m4:55:ARG:NH2   | 50:m4:76:ALA:O    | 2.05                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:d3:23:ARG:HG3  | 25:d3:23:ARG:HH11  | 1.37                     | 0.90              |
| 36:5:3182:G:OP1   | 52:m6:160:ARG:NH2  | 2.05                     | 0.90              |
| 1:6:1385:G:N7     | 86:6:2122:OHX:N6   | 2.20                     | 0.90              |
| 36:1:837:A:OP2    | 79:Q3:4:ARG:NH1    | 2.05                     | 0.90              |
| 1:6:1588:G:H1     | 1:6:1608:U:H3      | 1.20                     | 0.90              |
| 86:5:3904:OHX:N6  | 38:8:16:G:O6       | 2.05                     | 0.90              |
| 23:D1:74:GLN:NE2  | 23:D1:81:ASN:O     | 2.05                     | 0.89              |
| 36:5:2836:C:H5    | 36:5:2852:C:H42    | 1.17                     | 0.89              |
| 38:8:21:C:OP1     | 41:l4:193:LYS:NZ   | 2.05                     | 0.89              |
| 65:n9:24:PRO:HG2  | 65:n9:26:THR:HG22  | 1.54                     | 0.89              |
| 47:m0:175:ASN:OD1 | 47:m0:176:LEU:N    | 2.05                     | 0.89              |
| 36:1:2208:A:N1    | 86:1:4047:OHX:N2   | 2.20                     | 0.89              |
| 40:L3:139:GLN:O   | 40:L3:141:GLY:N    | 2.06                     | 0.89              |
| 1:2:79:C:H1'      | 8:S6:174:LYS:HD3   | 1.55                     | 0.89              |
| 1:6:1330:G:H21    | 19:c7:8:THR:HG21   | 1.36                     | 0.89              |
| 36:1:687:U:OP2    | 49:M3:36:ARG:NH2   | 2.05                     | 0.89              |
| 8:S6:163:THR:HG22 | 8:S6:168:THR:HG22  | 1.53                     | 0.88              |
| 54:M8:170:ARG:NH1 | 64:N8:56:VAL:O     | 2.07                     | 0.88              |
| 36:5:3272:C:OP2   | 43:l6:78:ARG:NH1   | 2.07                     | 0.88              |
| 48:m1:94:ARG:O    | 48:m1:96:PHE:N     | 2.07                     | 0.88              |
| 36:1:1233:G:H1    | 36:1:1255:C:H42    | 1.20                     | 0.88              |
| 21:c9:57:ARG:HG3  | 21:c9:57:ARG:HH11  | 1.39                     | 0.88              |
| 36:5:1875:G:H2'   | 36:5:1876:U:H5''   | 1.54                     | 0.87              |
| 36:1:3344:A:H2    | 36:1:3361:G:H21    | 1.20                     | 0.87              |
| 36:1:1222:G:HO2'  | 36:1:1285:G:H1     | 1.17                     | 0.87              |
| 36:5:3153:U:H4'   | 36:5:3154:C:H5'    | 1.57                     | 0.87              |
| 36:1:1639:C:OP2   | 70:O4:74:ARG:NH2   | 2.07                     | 0.87              |
| 78:Q2:17:CYS:SG   | 87:Q2:501:ZN:ZN    | 1.62                     | 0.87              |
| 41:L4:317:PRO:O   | 41:L4:319:LYS:N    | 2.07                     | 0.87              |
| 1:6:1696:G:O2'    | 1:6:1698:G:N7      | 2.06                     | 0.86              |
| 1:6:1552:U:OP2    | 17:c5:43:ARG:NH2   | 2.08                     | 0.86              |
| 39:L2:209:HIS:HD2 | 39:L2:211:HIS:H    | 1.22                     | 0.86              |
| 86:1:3962:OHX:N4  | 44:L7:217:PRO:HA   | 1.91                     | 0.86              |
| 1:2:68:A:OP1      | 8:S6:160:ARG:NH2   | 2.08                     | 0.86              |
| 36:1:2836:C:H5    | 36:1:2852:C:H42    | 1.23                     | 0.86              |
| 36:1:3166:C:H42   | 36:1:3284:G:H1     | 1.21                     | 0.86              |
| 40:l3:291:GLU:OE1 | 40:l3:302:LYS:NZ   | 2.08                     | 0.86              |
| 11:S9:93:LEU:HA   | 11:S9:96:VAL:HG13  | 1.57                     | 0.86              |
| 15:c3:114:ARG:HG2 | 15:c3:114:ARG:HH11 | 1.39                     | 0.86              |
| 3:S1:181:LEU:O    | 3:S1:185:THR:N     | 2.09                     | 0.86              |
| 36:1:3272:C:OP2   | 43:L6:78:ARG:NH1   | 2.08                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1654:A:H2'    | 36:5:1655:G:H5''   | 1.57                     | 0.86              |
| 16:C4:85:ALA:H     | 16:C4:119:THR:HG22 | 1.37                     | 0.86              |
| 36:1:2960:C:OP1    | 86:1:4005:OHX:N4   | 2.09                     | 0.86              |
| 36:1:3182:G:OP1    | 52:M6:160:ARG:NH2  | 2.08                     | 0.86              |
| 36:5:1078:U:O4     | 86:5:3999:OHX:N5   | 2.09                     | 0.86              |
| 36:5:3230:G:H4'    | 50:m4:132:LYS:HD3  | 1.57                     | 0.86              |
| 47:m0:77:THR:HG22  | 47:m0:82:ARG:HA    | 1.57                     | 0.86              |
| 1:2:1010:C:OP2     | 86:2:2132:OHX:N6   | 2.09                     | 0.86              |
| 36:5:2854:U:OP2    | 47:m0:3:ARG:NH2    | 2.08                     | 0.86              |
| 19:C7:47:ARG:NH1   | 19:C7:48:ASN:OD1   | 2.09                     | 0.85              |
| 1:2:9:U:O4         | 86:2:2156:OHX:N6   | 2.09                     | 0.85              |
| 1:2:740:A:H2'      | 1:2:741:C:H5''     | 1.57                     | 0.85              |
| 36:5:272:G:OP2     | 86:5:4074:OHX:N6   | 2.09                     | 0.85              |
| 36:5:1613:A:OP2    | 74:o8:46:ARG:NH2   | 2.09                     | 0.85              |
| 10:S8:162:ALA:HA   | 36:1:3353:G:H5'    | 1.58                     | 0.85              |
| 6:s4:9:LEU:HB2     | 6:s4:30:ARG:HB2    | 1.58                     | 0.85              |
| 2:S0:179:ARG:HD3   | 2:S0:183:ARG:HH11  | 1.41                     | 0.85              |
| 38:4:70:G:O6       | 86:O7:103:OHX:N4   | 2.10                     | 0.85              |
| 17:C5:126:VAL:HG13 | 17:C5:127:ARG:H    | 1.40                     | 0.85              |
| 53:m7:69:ARG:HG2   | 53:m7:79:THR:HG23  | 1.56                     | 0.85              |
| 71:O5:101:THR:HG22 | 71:O5:104:GLN:H    | 1.42                     | 0.84              |
| 41:l4:16:THR:HG22  | 41:l4:18:ASN:H     | 1.41                     | 0.84              |
| 36:1:2123:G:N7     | 86:1:4201:OHX:N2   | 2.26                     | 0.84              |
| 26:D4:8:ARG:NH1    | 26:D4:26:ASP:OD1   | 2.11                     | 0.84              |
| 10:s8:62:THR:HA    | 10:s8:76:THR:O     | 1.78                     | 0.84              |
| 36:5:1073:U:H1'    | 65:n9:50:THR:HG22  | 1.58                     | 0.84              |
| 1:2:895:G:H1       | 1:2:917:U:H3       | 1.23                     | 0.84              |
| 1:2:142:G:H22      | 1:2:173:A:H2       | 1.25                     | 0.84              |
| 10:s8:34:ALA:HB2   | 10:s8:56:ARG:HD3   | 1.58                     | 0.83              |
| 36:5:2311:G:OP2    | 86:5:4196:OHX:N1   | 2.11                     | 0.83              |
| 3:S1:201:THR:HG21  | 3:S1:207:LEU:HD22  | 1.58                     | 0.83              |
| 13:c1:132:SER:O    | 13:c1:134:THR:N    | 2.10                     | 0.83              |
| 37:3:49:G:N7       | 42:L5:58:LYS:HG3   | 1.92                     | 0.83              |
| 2:S0:83:GLN:HG2    | 2:S0:99:ALA:HB1    | 1.60                     | 0.83              |
| 55:M9:27:ASN:O     | 86:M9:202:OHX:N6   | 2.11                     | 0.83              |
| 1:6:1010:C:OP2     | 86:6:2171:OHX:N3   | 2.12                     | 0.83              |
| 78:Q2:73:GLU:OE1   | 78:Q2:80:ARG:NH2   | 2.10                     | 0.83              |
| 77:q1:9:ARG:HH11   | 77:q1:9:ARG:HG3    | 1.43                     | 0.83              |
| 1:2:732:G:O6       | 86:2:2130:OHX:N5   | 2.10                     | 0.83              |
| 53:M7:109:ALA:HA   | 53:M7:112:LEU:HD22 | 1.59                     | 0.83              |
| 63:N7:135:ARG:HG2  | 63:N7:135:ARG:HH21 | 1.44                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 64:N8:6:THR:HG23   | 64:N8:8:THR:HG23  | 1.61                     | 0.83              |
| 1:6:280:U:OP2      | 60:n4:113:LYS:NZ  | 2.10                     | 0.83              |
| 36:1:2940:A:N7     | 40:L3:2:SER:N     | 2.27                     | 0.82              |
| 41:l4:300:ARG:O    | 54:m8:39:ARG:NH1  | 2.11                     | 0.82              |
| 1:2:1385:G:N7      | 86:2:2133:OHX:N3  | 2.25                     | 0.82              |
| 10:S8:36:THR:HG21  | 10:S8:173:PRO:HB2 | 1.61                     | 0.82              |
| 1:6:475:A:OP2      | 11:s9:126:ARG:NH1 | 2.12                     | 0.82              |
| 1:2:992:A:H2       | 1:2:1012:U:H3     | 1.25                     | 0.82              |
| 59:N3:40:LYS:HE2   | 59:N3:59:MET:HE3  | 1.62                     | 0.82              |
| 1:6:1726:G:N7      | 86:6:2147:OHX:N5  | 2.28                     | 0.82              |
| 18:C6:40:GLU:HA    | 18:C6:42:GLU:H    | 1.43                     | 0.82              |
| 40:l3:347:SER:HB3  | 40:l3:350:ALA:H   | 1.43                     | 0.82              |
| 1:2:140:A:N6       | 1:2:281:G:OP1     | 2.12                     | 0.82              |
| 36:1:3214:U:OP2    | 50:M4:128:ARG:NH2 | 2.11                     | 0.82              |
| 1:6:755:A:O2'      | 1:6:756:A:O4'     | 1.98                     | 0.82              |
| 1:6:1041:G:OP1     | 86:6:2175:OHX:N4  | 2.13                     | 0.82              |
| 40:l3:76:VAL:HG11  | 40:l3:323:MET:HE3 | 1.62                     | 0.82              |
| 44:l7:134:VAL:O    | 44:l7:229:PHE:HA  | 1.80                     | 0.82              |
| 36:5:658:G:OP1     | 86:5:4092:OHX:N5  | 2.12                     | 0.82              |
| 78:q2:48:SER:O     | 86:q2:502:OHX:N3  | 2.13                     | 0.82              |
| 40:l3:37:ARG:HG2   | 40:l3:187:SER:H   | 1.45                     | 0.82              |
| 36:1:2794:G:N7     | 86:1:3938:OHX:N2  | 2.27                     | 0.82              |
| 1:6:471:A:OP2      | 86:6:2103:OHX:N5  | 2.13                     | 0.82              |
| 36:5:368:G:OP1     | 86:5:3924:OHX:N4  | 2.13                     | 0.82              |
| 28:D6:79:ILE:HA    | 28:D6:84:VAL:HB   | 1.62                     | 0.81              |
| 36:1:1814:A:H4'    | 36:1:1815:U:H5'   | 1.62                     | 0.81              |
| 42:L5:40:HIS:HD2   | 42:L5:42:ALA:H    | 1.28                     | 0.81              |
| 46:L9:22:SER:OG    | 46:L9:23:ARG:N    | 2.11                     | 0.81              |
| 1:2:237:C:H5''     | 1:2:238:U:H5'     | 1.61                     | 0.81              |
| 1:6:161:U:OP2      | 8:s6:87:ARG:NH2   | 2.13                     | 0.81              |
| 36:5:2174:G:OP2    | 39:l2:193:ARG:NH1 | 2.13                     | 0.81              |
| 36:1:2895:G:H2'    | 36:1:2896:A:H5''  | 1.62                     | 0.81              |
| 3:s1:70:LEU:HB3    | 3:s1:79:HIS:HB3   | 1.62                     | 0.81              |
| 22:d0:53:LYS:HB2   | 22:d0:92:ASP:HB2  | 1.62                     | 0.81              |
| 41:l4:329:PRO:O    | 41:l4:331:ALA:N   | 2.13                     | 0.81              |
| 1:6:990:C:OP2      | 86:6:2121:OHX:N2  | 2.12                     | 0.81              |
| 1:6:1521:G:O6      | 21:c9:68:ARG:NH1  | 2.13                     | 0.81              |
| 75:o9:5:LYS:HD3    | 75:o9:13:MET:HE1  | 1.58                     | 0.81              |
| 1:2:475:A:OP2      | 11:S9:126:ARG:NH1 | 2.13                     | 0.81              |
| 48:M1:94:ARG:O     | 48:M1:96:PHE:N    | 2.11                     | 0.81              |
| 34:sR:184:ASN:HD22 | 34:sR:185:GLN:H   | 1.29                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:e0:59:GLY:O     | 80:e0:61:SER:N     | 2.14                     | 0.81              |
| 3:S1:70:LEU:HA     | 3:S1:73:LEU:HB3    | 1.63                     | 0.81              |
| 36:1:1213:G:H4'    | 56:N0:90:MET:HG2   | 1.63                     | 0.81              |
| 53:M7:62:ARG:O     | 86:M7:207:OHX:N1   | 2.14                     | 0.81              |
| 27:d5:38:HIS:HA    | 27:d5:70:LYS:HD3   | 1.63                     | 0.81              |
| 42:l5:120:LYS:O    | 42:l5:248:ARG:NH2  | 2.13                     | 0.81              |
| 18:C6:82:ARG:HH22  | 18:C6:114:ARG:HB2  | 1.45                     | 0.81              |
| 63:n7:88:ASP:O     | 63:n7:121:ARG:NH2  | 2.12                     | 0.81              |
| 10:S8:103:GLN:HB3  | 10:S8:164:ARG:HG2  | 1.63                     | 0.80              |
| 63:N7:46:ILE:HD13  | 63:N7:68:ILE:HG23  | 1.63                     | 0.80              |
| 41:L4:145:ILE:HD11 | 41:L4:148:ILE:HG13 | 1.62                     | 0.80              |
| 36:5:2255:A:H5'    | 36:5:2261:G:H22    | 1.46                     | 0.80              |
| 36:1:1898:G:OP2    | 86:1:3935:OHX:N4   | 2.15                     | 0.80              |
| 3:s1:62:LYS:O      | 3:s1:64:ARG:N      | 2.14                     | 0.80              |
| 36:5:2233:A:OP2    | 86:5:3962:OHX:N5   | 2.14                     | 0.80              |
| 1:2:991:G:OP2      | 86:2:2132:OHX:N1   | 2.15                     | 0.80              |
| 56:N0:23:LYS:O     | 57:N1:146:ASN:ND2  | 2.10                     | 0.80              |
| 1:6:1429:G:H1'     | 22:d0:74:GLU:HG2   | 1.64                     | 0.80              |
| 44:l7:88:ARG:HD2   | 44:l7:90:LYS:O     | 1.80                     | 0.80              |
| 36:1:770:G:N7      | 86:1:4099:OHX:N6   | 2.30                     | 0.80              |
| 10:s8:36:THR:HG21  | 10:s8:173:PRO:HB2  | 1.62                     | 0.80              |
| 71:o5:101:THR:HG22 | 71:o5:104:GLN:H    | 1.47                     | 0.80              |
| 1:2:1202:A:OP1     | 86:2:2111:OHX:N1   | 2.15                     | 0.80              |
| 42:L5:233:ALA:O    | 42:L5:235:SER:N    | 2.14                     | 0.80              |
| 1:6:647:G:N2       | 1:6:687:G:H22      | 1.79                     | 0.80              |
| 1:6:755:A:H2'      | 1:6:756:A:C8       | 2.16                     | 0.80              |
| 41:l4:338:LYS:O    | 41:l4:340:GLY:N    | 2.14                     | 0.80              |
| 36:1:2767:U:O2'    | 78:Q2:30:ALA:O     | 1.99                     | 0.80              |
| 73:O7:87:SER:O     | 86:O7:103:OHX:N3   | 2.14                     | 0.80              |
| 2:s0:9:LEU:HD11    | 2:s0:14:ALA:HB2    | 1.64                     | 0.80              |
| 8:s6:153:VAL:O     | 8:s6:155:ASP:N     | 2.14                     | 0.80              |
| 52:m6:110:PRO:O    | 52:m6:112:TYR:N    | 2.15                     | 0.80              |
| 61:N5:115:ARG:HG3  | 61:N5:115:ARG:HH11 | 1.45                     | 0.80              |
| 1:6:895:G:H21      | 16:c4:38:THR:HG21  | 1.47                     | 0.80              |
| 26:d4:29:HIS:HB3   | 26:d4:32:ARG:HB2   | 1.64                     | 0.80              |
| 86:5:4187:OHX:N2   | 72:o6:28:TYR:O     | 2.15                     | 0.80              |
| 25:D3:102:VAL:HG12 | 25:D3:127:VAL:HG12 | 1.64                     | 0.80              |
| 1:6:755:A:H2'      | 1:6:756:A:H8       | 1.45                     | 0.80              |
| 7:s5:92:ARG:HG2    | 7:s5:92:ARG:HH11   | 1.47                     | 0.80              |
| 46:l9:20:ILE:HD13  | 46:l9:25:VAL:HG22  | 1.63                     | 0.80              |
| 13:C1:99:ARG:NH1   | 25:D3:7:ARG:O      | 2.15                     | 0.79              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:L9:105:GLU:HA  | 46:L9:109:ALA:HB3 | 1.65                     | 0.79              |
| 36:5:2620:G:O6    | 86:5:4241:OHX:N4  | 2.15                     | 0.79              |
| 86:5:4002:OHX:N5  | 44:17:217:PRO:HA  | 1.97                     | 0.79              |
| 36:1:317:A:OP2    | 72:O6:30:LYS:NZ   | 2.15                     | 0.79              |
| 1:6:1097:U:H4'    | 1:6:1098:U:H5'    | 1.63                     | 0.79              |
| 1:2:1521:G:O6     | 21:C9:68:ARG:NH1  | 2.16                     | 0.79              |
| 6:s4:100:ARG:HG2  | 6:s4:102:VAL:HG12 | 1.64                     | 0.79              |
| 62:n6:45:ILE:HD11 | 62:n6:122:LYS:HB2 | 1.65                     | 0.79              |
| 4:S2:82:ASN:HD22  | 4:S2:207:LEU:HD13 | 1.47                     | 0.79              |
| 1:2:1429:G:H1'    | 22:D0:74:GLU:HG2  | 1.62                     | 0.79              |
| 47:M0:193:ASP:OD2 | 47:M0:194:GLY:N   | 2.16                     | 0.79              |
| 2:s0:62:ARG:HG3   | 2:s0:62:ARG:HH11  | 1.46                     | 0.79              |
| 36:1:830:A:OP1    | 86:1:4014:OHX:N4  | 2.16                     | 0.79              |
| 2:s0:41:ARG:HH11  | 2:s0:45:VAL:HG21  | 1.48                     | 0.79              |
| 53:m7:122:ALA:HB3 | 53:m7:143:PRO:HB2 | 1.65                     | 0.79              |
| 1:2:1291:G:H5'    | 4:S2:119:LYS:HE2  | 1.63                     | 0.79              |
| 63:N7:15:ARG:NH2  | 70:O4:83:ASN:OD1  | 2.15                     | 0.79              |
| 36:1:329:U:OP2    | 86:1:4046:OHX:N4  | 2.16                     | 0.78              |
| 71:o5:78:LYS:HA   | 71:o5:81:ARG:HD3  | 1.64                     | 0.78              |
| 1:2:471:A:OP2     | 86:2:2077:OHX:N4  | 2.17                     | 0.78              |
| 1:2:701:U:H3      | 1:2:737:A:H61     | 1.30                     | 0.78              |
| 1:2:1203:A:OP2    | 86:2:2111:OHX:N5  | 2.16                     | 0.78              |
| 7:S5:57:SER:O     | 7:S5:59:VAL:N     | 2.16                     | 0.78              |
| 1:6:453:U:O4      | 86:6:2062:OHX:N4  | 2.16                     | 0.78              |
| 36:1:2356:A:H61   | 36:1:2983:C:H5    | 1.28                     | 0.78              |
| 1:6:1765:A:OP1    | 86:6:2126:OHX:N2  | 2.17                     | 0.78              |
| 42:l5:4:GLN:NE2   | 42:l5:4:GLN:O     | 2.16                     | 0.78              |
| 70:o4:41:ARG:HA   | 70:o4:56:THR:HG22 | 1.66                     | 0.78              |
| 2:S0:41:ARG:HE    | 2:S0:45:VAL:HB    | 1.48                     | 0.78              |
| 5:S3:7:LYS:NZ     | 22:D0:115:GLU:OE2 | 2.17                     | 0.78              |
| 37:7:1:G:O2'      | 42:l5:270:LYS:HB3 | 1.84                     | 0.78              |
| 29:D7:29:ARG:HH11 | 29:D7:29:ARG:HG3  | 1.48                     | 0.78              |
| 38:4:62:C:O2      | 86:4:227:OHX:N5   | 2.17                     | 0.78              |
| 36:5:2398:A:H5'   | 36:5:2398:A:H8    | 1.49                     | 0.78              |
| 1:2:1681:A:H2'    | 1:2:1682:U:H5'    | 1.66                     | 0.78              |
| 4:S2:69:ILE:HD11  | 4:S2:133:LYS:HG2  | 1.65                     | 0.78              |
| 36:1:819:U:OP1    | 73:O7:10:LYS:NZ   | 2.14                     | 0.78              |
| 36:1:1740:U:H1'   | 36:1:1741:A:H2    | 1.49                     | 0.78              |
| 1:6:1280:C:H2'    | 1:6:1281:G:H8     | 1.49                     | 0.78              |
| 1:6:1695:G:H21    | 1:6:1706:C:H41    | 1.28                     | 0.78              |
| 4:S2:147:ASN:HB3  | 23:D1:4:ASP:HA    | 1.64                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:m7:25:SER:O     | 53:m7:29:THR:HG23  | 1.82                     | 0.78              |
| 34:SR:170:ILE:HG21 | 34:SR:211:ILE:HD11 | 1.64                     | 0.78              |
| 40:L3:171:LEU:O    | 86:L3:403:OHX:N6   | 2.17                     | 0.78              |
| 36:5:2971:A:H3'    | 36:5:2971:A:N3     | 1.99                     | 0.78              |
| 1:2:702:G:O6       | 1:2:736:C:N4       | 2.14                     | 0.77              |
| 51:M5:68:ARG:HG2   | 51:M5:68:ARG:HH11  | 1.49                     | 0.77              |
| 36:5:1427:U:OP2    | 64:n8:4:ARG:NH2    | 2.18                     | 0.77              |
| 36:5:1565:G:N1     | 36:5:1574:C:N3     | 2.32                     | 0.77              |
| 1:2:320:U:H3'      | 1:2:321:C:H5''     | 1.65                     | 0.77              |
| 8:S6:67:VAL:HG21   | 8:S6:99:GLY:HA2    | 1.66                     | 0.77              |
| 36:1:776:U:H5      | 36:1:2719:U:O2     | 1.67                     | 0.77              |
| 1:6:301:A:OP2      | 86:6:2093:OHX:N1   | 2.18                     | 0.77              |
| 6:s4:79:ASP:HB3    | 6:s4:82:TYR:HB2    | 1.65                     | 0.77              |
| 57:n1:51:GLY:HA3   | 57:n1:92:ARG:HG3   | 1.65                     | 0.77              |
| 5:S3:7:LYS:HE2     | 22:D0:27:THR:HG21  | 1.65                     | 0.77              |
| 41:L4:300:ARG:O    | 54:M8:39:ARG:NH1   | 2.18                     | 0.77              |
| 46:L9:8:GLN:HG2    | 46:L9:68:LEU:HD13  | 1.64                     | 0.77              |
| 38:8:95:G:OP2      | 73:o7:72:ARG:NH1   | 2.17                     | 0.77              |
| 78:q2:50:PHE:O     | 86:q2:502:OHX:N1   | 2.18                     | 0.77              |
| 36:1:300:G:O6      | 86:1:4153:OHX:N1   | 2.17                     | 0.77              |
| 44:L7:163:LEU:O    | 44:L7:165:ASP:N    | 2.17                     | 0.77              |
| 1:6:513:U:OP1      | 11:s9:133:HIS:NE2  | 2.13                     | 0.77              |
| 1:6:1665:U:O4      | 86:6:2124:OHX:N6   | 2.17                     | 0.77              |
| 39:l2:147:ARG:HH22 | 39:l2:155:LYS:HG3  | 1.49                     | 0.77              |
| 46:l9:166:ARG:HH21 | 46:l9:168:ARG:HH12 | 1.30                     | 0.77              |
| 54:m8:158:HIS:H    | 54:m8:186:VAL:HG12 | 1.49                     | 0.77              |
| 49:m3:166:ALA:HB1  | 64:n8:147:LEU:HD21 | 1.64                     | 0.77              |
| 25:D3:91:GLY:O     | 25:D3:93:LEU:N     | 2.17                     | 0.77              |
| 50:M4:113:THR:HG22 | 50:M4:116:GLU:H    | 1.48                     | 0.77              |
| 36:5:2818:U:H5'    | 36:5:2818:U:H6     | 1.48                     | 0.77              |
| 11:s9:3:ARG:HG2    | 11:s9:3:ARG:HH21   | 1.49                     | 0.77              |
| 36:5:744:A:OP1     | 54:m8:66:ARG:NH2   | 2.18                     | 0.77              |
| 1:2:348:U:O4       | 86:2:2128:OHX:N5   | 2.17                     | 0.77              |
| 5:S3:108:LYS:HG2   | 5:S3:113:LEU:HD12  | 1.67                     | 0.77              |
| 7:S5:216:GLU:OE2   | 7:S5:219:ARG:NH2   | 2.16                     | 0.77              |
| 34:SR:161:LYS:O    | 34:SR:161:LYS:HG2  | 1.83                     | 0.77              |
| 36:1:356:C:OP2     | 86:O9:101:OHX:N1   | 2.17                     | 0.77              |
| 36:1:1110:U:H2'    | 36:1:1111:U:C6     | 2.20                     | 0.77              |
| 47:M0:24:ARG:HH11  | 47:M0:24:ARG:HG3   | 1.49                     | 0.77              |
| 53:M7:25:SER:O     | 53:M7:29:THR:HG23  | 1.84                     | 0.77              |
| 1:2:127:G:N7       | 8:S6:202:ARG:NH2   | 2.32                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:O2:91:THR:HG22  | 68:O2:92:TYR:CD2   | 2.20                     | 0.77              |
| 21:c9:105:LEU:HD13 | 21:c9:122:ARG:HD3  | 1.66                     | 0.77              |
| 40:l3:296:THR:HG22 | 40:l3:298:PHE:N    | 1.97                     | 0.77              |
| 86:2:2032:OHX:N4   | 86:2:2147:OHX:N2   | 2.33                     | 0.77              |
| 28:D6:37:LYS:O     | 28:D6:38:ARG:NH1   | 2.16                     | 0.77              |
| 42:l5:270:LYS:HG3  | 42:l5:273:ARG:HB3  | 1.64                     | 0.77              |
| 47:m0:117:GLY:O    | 86:m0:302:OHX:N6   | 2.18                     | 0.77              |
| 36:1:662:U:OP1     | 64:N8:8:THR:HG21   | 1.85                     | 0.76              |
| 48:M1:23:VAL:O     | 48:M1:25:GLU:N     | 2.17                     | 0.76              |
| 1:6:1253:U:O4      | 33:e1:97:LYS:NZ    | 2.16                     | 0.76              |
| 36:5:2975:U:OP1    | 86:5:4089:OHX:N3   | 2.17                     | 0.76              |
| 36:5:3068:U:OP2    | 55:m9:62:ARG:NH2   | 2.17                     | 0.76              |
| 51:m5:31:ARG:NH1   | 51:m5:124:ASP:OD1  | 2.18                     | 0.76              |
| 56:N0:91:TYR:O     | 56:N0:137:ARG:NH1  | 2.19                     | 0.76              |
| 22:d0:27:THR:HB    | 22:d0:88:LYS:HG2   | 1.66                     | 0.76              |
| 1:2:1459:C:OP1     | 20:C8:126:ARG:NH2  | 2.18                     | 0.76              |
| 3:S1:77:GLU:OE1    | 16:C4:114:ARG:NH2  | 2.18                     | 0.76              |
| 6:S4:139:VAL:HG13  | 6:S4:150:PRO:HG3   | 1.67                     | 0.76              |
| 36:1:1940:G:H21    | 36:1:3362:A:H8     | 1.33                     | 0.76              |
| 69:O3:48:ARG:HG2   | 69:O3:48:ARG:NH1   | 1.99                     | 0.76              |
| 36:5:2915:U:C5     | 40:l3:7:GLU:HG2    | 2.21                     | 0.76              |
| 10:S8:36:THR:HB    | 10:S8:57:ALA:O     | 1.86                     | 0.76              |
| 36:1:1196:C:O2     | 86:3:218:OHX:N2    | 2.17                     | 0.76              |
| 1:6:1774:G:N7      | 77:q1:4:LYS:NZ     | 2.33                     | 0.76              |
| 73:o7:25:ARG:HB3   | 73:o7:25:ARG:HH11  | 1.51                     | 0.76              |
| 50:M4:55:ARG:NH2   | 50:M4:76:ALA:O     | 2.18                     | 0.76              |
| 1:6:542:A:C8       | 1:6:543:C:H2'      | 2.21                     | 0.76              |
| 49:m3:113:VAL:HG12 | 49:m3:117:LYS:HD2  | 1.68                     | 0.76              |
| 64:n8:77:LYS:O     | 64:n8:79:TRP:N     | 2.19                     | 0.76              |
| 64:n8:82:ILE:HD11  | 64:n8:102:ILE:HG12 | 1.66                     | 0.76              |
| 1:2:1479:A:OP1     | 21:C9:57:ARG:NH1   | 2.19                     | 0.76              |
| 1:6:151:G:H1       | 1:6:163:G:H1       | 1.33                     | 0.76              |
| 64:n8:6:THR:HG23   | 64:n8:8:THR:HG23   | 1.67                     | 0.76              |
| 41:L4:152:VAL:HG23 | 41:L4:172:VAL:HG21 | 1.67                     | 0.76              |
| 71:O5:78:LYS:HA    | 71:O5:81:ARG:HD3   | 1.68                     | 0.76              |
| 25:d3:125:VAL:HG12 | 25:d3:126:LYS:HG3  | 1.66                     | 0.76              |
| 1:2:104:A:OP2      | 1:2:308:C:N4       | 2.18                     | 0.76              |
| 1:2:1542:G:N2      | 1:2:1569:A:OP2     | 2.18                     | 0.76              |
| 16:C4:13:VAL:HG13  | 16:C4:77:THR:H     | 1.50                     | 0.76              |
| 27:D5:41:ILE:HG23  | 27:D5:42:LEU:H     | 1.51                     | 0.76              |
| 41:L4:16:THR:HG22  | 41:L4:18:ASN:H     | 1.51                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:s3:7:LYS:HE3     | 22:d0:27:THR:HG21  | 1.67                     | 0.76              |
| 11:s9:59:LEU:HD22  | 11:s9:69:ARG:HA    | 1.67                     | 0.76              |
| 19:c7:27:ASP:O     | 19:c7:31:ASN:ND2   | 2.19                     | 0.76              |
| 36:1:670:C:OP1     | 54:M8:147:ARG:NH2  | 2.16                     | 0.76              |
| 36:1:3375:A:O2'    | 36:1:3378:C:OP2    | 2.03                     | 0.76              |
| 1:6:1502:G:N7      | 21:c9:102:ARG:NH2  | 2.34                     | 0.76              |
| 41:L4:232:SER:OG   | 41:L4:233:LEU:N    | 2.15                     | 0.75              |
| 63:n7:33:SER:OG    | 63:n7:35:SER:O     | 2.04                     | 0.75              |
| 86:2:2032:OHX:N4   | 86:2:2147:OHX:N1   | 2.34                     | 0.75              |
| 36:5:1381:A:OP1    | 41:l4:197:ARG:NH1  | 2.19                     | 0.75              |
| 66:o0:101:LEU:HD22 | 66:o0:101:LEU:H    | 1.51                     | 0.75              |
| 1:2:1508:U:O4      | 86:2:2032:OHX:N5   | 2.19                     | 0.75              |
| 24:D2:27:ILE:HG12  | 24:D2:61:ILE:HB    | 1.66                     | 0.75              |
| 39:L2:96:LEU:HD22  | 79:Q3:83:ILE:HG23  | 1.67                     | 0.75              |
| 36:5:776:U:H5      | 36:5:2719:U:O2     | 1.68                     | 0.75              |
| 36:5:3276:G:H2'    | 36:5:3276:G:OP2    | 1.86                     | 0.75              |
| 47:m0:84:ALA:O     | 47:m0:140:THR:HG22 | 1.85                     | 0.75              |
| 1:2:579:A:H2       | 5:S3:143:ARG:HG3   | 1.51                     | 0.75              |
| 13:C1:4:GLU:HG2    | 13:C1:5:LEU:HG     | 1.66                     | 0.75              |
| 20:C8:30:TYR:HE2   | 20:C8:40:ARG:HH11  | 1.30                     | 0.75              |
| 71:O5:85:THR:HG22  | 71:O5:88:LEU:H     | 1.50                     | 0.75              |
| 72:O6:2:THR:OG1    | 72:O6:3:VAL:N      | 2.20                     | 0.75              |
| 7:s5:94:THR:HG22   | 7:s5:114:ILE:HG13  | 1.69                     | 0.75              |
| 1:2:1720:G:O6      | 86:2:2083:OHX:N5   | 2.20                     | 0.75              |
| 11:s9:64:GLU:OE1   | 11:s9:69:ARG:NH2   | 2.19                     | 0.75              |
| 40:l3:139:GLN:HB2  | 40:l3:141:GLY:H    | 1.51                     | 0.75              |
| 35:SM:23:LYS:H     | 35:SM:23:LYS:HD2   | 1.51                     | 0.75              |
| 36:1:2771:U:O2'    | 36:1:2772:C:O4'    | 2.04                     | 0.75              |
| 64:N8:94:ALA:HB1   | 64:N8:121:VAL:HA   | 1.69                     | 0.75              |
| 36:1:2392:C:O2'    | 40:L3:266:ARG:NH2  | 2.18                     | 0.75              |
| 58:N2:51:GLY:O     | 58:N2:52:ASN:ND2   | 2.17                     | 0.75              |
| 2:s0:70:PRO:HB2    | 2:s0:94:GLY:HA3    | 1.68                     | 0.75              |
| 1:2:820:U:H2'      | 1:2:821:U:H4'      | 1.67                     | 0.75              |
| 41:L4:60:THR:HG21  | 41:L4:77:VAL:HG22  | 1.68                     | 0.75              |
| 1:2:770:A:OP2      | 86:2:2139:OHX:N6   | 2.20                     | 0.75              |
| 1:2:1572:G:H1'     | 7:S5:185:ARG:HH12  | 1.52                     | 0.75              |
| 41:L4:291:ASN:O    | 41:L4:293:SER:N    | 2.20                     | 0.75              |
| 81:m2:120:UNK:O    | 81:m2:122:UNK:N    | 2.20                     | 0.75              |
| 1:2:1370:U:O4      | 86:2:2121:OHX:N1   | 2.19                     | 0.74              |
| 9:S7:11:GLN:HG3    | 9:S7:13:PRO:HD2    | 1.68                     | 0.74              |
| 37:3:60:G:OP2      | 86:3:226:OHX:N3    | 2.20                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:O0:63:SER:HG    | 66:O0:65:THR:HG1   | 1.28                     | 0.74              |
| 36:5:1541:G:OP2    | 86:5:4093:OHX:N4   | 2.20                     | 0.74              |
| 71:o5:85:THR:HG22  | 71:o5:88:LEU:H     | 1.52                     | 0.74              |
| 8:S6:33:GLY:HA2    | 8:S6:51:LYS:HE2    | 1.66                     | 0.74              |
| 1:6:65:A:H2        | 1:6:84:A:H62       | 1.36                     | 0.74              |
| 36:5:2236:G:OP1    | 86:5:4247:OHX:N3   | 2.20                     | 0.74              |
| 43:l6:31:ARG:HH11  | 69:o3:107:ILE:HG22 | 1.51                     | 0.74              |
| 15:C3:142:GLU:HB2  | 15:C3:145:THR:HG23 | 1.69                     | 0.74              |
| 51:M5:38:ARG:HG3   | 51:M5:38:ARG:HH11  | 1.53                     | 0.74              |
| 25:D3:69:ARG:NH1   | 25:D3:116:ASP:OD1  | 2.19                     | 0.74              |
| 36:1:2513:U:H2'    | 36:1:2592:G:H1     | 1.53                     | 0.74              |
| 1:6:1681:A:H2      | 1:6:1720:G:H21     | 1.33                     | 0.74              |
| 41:l4:226:GLU:OE1  | 41:l4:237:GLN:NE2  | 2.20                     | 0.74              |
| 36:1:3118:C:H4'    | 76:Q0:106:ARG:HH22 | 1.52                     | 0.74              |
| 18:c6:95:LYS:HE3   | 18:c6:96:TYR:CZ    | 2.23                     | 0.74              |
| 36:1:408:A:OP1     | 86:1:4060:OHX:N3   | 2.21                     | 0.74              |
| 36:1:2532:U:O4     | 36:1:2547:A:N6     | 2.19                     | 0.74              |
| 37:3:44:C:OP2      | 48:M1:137:ARG:NH2  | 2.20                     | 0.74              |
| 71:O5:10:ARG:NH1   | 71:O5:60:GLU:OE1   | 2.21                     | 0.74              |
| 1:6:1150:G:O6      | 86:6:2115:OHX:N5   | 2.20                     | 0.74              |
| 36:5:1065:A:N1     | 65:n9:26:THR:OG1   | 2.19                     | 0.74              |
| 36:5:3115:C:OP1    | 46:l9:62:ARG:NH2   | 2.21                     | 0.74              |
| 86:2:2032:OHX:N3   | 86:2:2147:OHX:N5   | 2.36                     | 0.74              |
| 3:s1:144:ARG:NH2   | 3:s1:207:LEU:O     | 2.21                     | 0.74              |
| 36:5:20:A:OP2      | 71:o5:90:ARG:NH1   | 2.21                     | 0.74              |
| 58:n2:42:LYS:HG2   | 58:n2:46:ALA:HA    | 1.69                     | 0.74              |
| 86:1:3962:OHX:N3   | 44:L7:217:PRO:O    | 2.21                     | 0.74              |
| 20:c8:134:ARG:O    | 20:c8:136:GLN:N    | 2.19                     | 0.74              |
| 51:M5:190:THR:O    | 51:M5:194:GLN:HG2  | 1.88                     | 0.73              |
| 55:M9:105:LEU:HD13 | 55:M9:135:LYS:HD2  | 1.70                     | 0.73              |
| 1:6:1595:U:H3      | 1:6:1600:A:H2      | 1.35                     | 0.73              |
| 75:o9:23:LEU:HD22  | 75:o9:24:PRO:HD2   | 1.70                     | 0.73              |
| 54:M8:158:HIS:H    | 54:M8:186:VAL:HG12 | 1.53                     | 0.73              |
| 1:6:959:U:H5''     | 29:d7:28:PRO:HB3   | 1.69                     | 0.73              |
| 36:5:2234:G:O6     | 86:5:3962:OHX:N1   | 2.21                     | 0.73              |
| 66:o0:18:ILE:HG22  | 66:o0:19:LYS:HD3   | 1.69                     | 0.73              |
| 4:S2:174:ARG:O     | 11:S9:53:ARG:NH2   | 2.21                     | 0.73              |
| 36:1:2255:A:H5'    | 36:1:2261:G:H22    | 1.53                     | 0.73              |
| 16:c4:87:GLY:HA3   | 16:c4:120:PRO:HG2  | 1.71                     | 0.73              |
| 49:m3:3:ILE:HG21   | 64:n8:45:MET:HE3   | 1.68                     | 0.73              |
| 1:2:1597:A:OP2     | 31:D9:32:ARG:NH2   | 2.20                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:924:G:OP1     | 86:1:4146:OHX:N5   | 2.21                     | 0.73              |
| 36:1:1240:A:H61    | 36:1:1244:A:H5''   | 1.53                     | 0.73              |
| 44:17:216:VAL:HG11 | 44:17:227:GLY:HA3  | 1.71                     | 0.73              |
| 10:S8:89:GLU:OE1   | 10:S8:92:ARG:NH2   | 2.19                     | 0.73              |
| 10:S8:197:THR:HA   | 10:S8:200:LYS:HB2  | 1.71                     | 0.73              |
| 35:SM:79:SER:HA    | 35:SM:82:THR:HG23  | 1.71                     | 0.73              |
| 36:1:3155:U:H3'    | 36:1:3156:U:H4'    | 1.71                     | 0.73              |
| 1:6:1479:A:OP1     | 21:c9:57:ARG:NH1   | 2.21                     | 0.73              |
| 53:m7:138:LYS:HG3  | 53:m7:140:GLU:HG3  | 1.71                     | 0.73              |
| 1:2:169:A:H5''     | 8:S6:176:GLN:HG2   | 1.69                     | 0.73              |
| 74:O8:66:ILE:HA    | 74:O8:69:LEU:HD23  | 1.69                     | 0.73              |
| 36:5:2201:G:H21    | 39:l2:224:THR:HG21 | 1.53                     | 0.73              |
| 36:5:3280:U:O2'    | 36:5:3281:U:H5''   | 1.89                     | 0.73              |
| 1:2:1520:U:OP2     | 21:C9:75:LYS:NZ    | 2.20                     | 0.73              |
| 1:2:1562:G:OP1     | 21:C9:89:ARG:NH2   | 2.21                     | 0.73              |
| 36:1:18:G:OP1      | 71:O5:81:ARG:NH2   | 2.19                     | 0.73              |
| 42:L5:56:THR:O     | 42:L5:58:LYS:N     | 2.19                     | 0.73              |
| 13:c1:94:ILE:HG12  | 25:d3:16:ARG:HD2   | 1.71                     | 0.73              |
| 46:l9:171:ASP:OD1  | 46:l9:173:ARG:HD3  | 1.89                     | 0.73              |
| 33:E1:108:VAL:HB   | 33:E1:114:VAL:HG22 | 1.70                     | 0.73              |
| 36:1:1724:U:H1'    | 36:1:1725:C:C6     | 2.24                     | 0.73              |
| 40:L3:173:GLN:O    | 40:L3:175:LYS:N    | 2.22                     | 0.73              |
| 1:6:783:G:OP2      | 26:d4:14:SER:OG    | 2.06                     | 0.73              |
| 1:6:1151:A:O2'     | 1:6:1766:A:N7      | 2.21                     | 0.73              |
| 1:6:1637:C:OP2     | 86:6:2115:OHX:N4   | 2.22                     | 0.73              |
| 18:c6:50:GLU:OE2   | 18:c6:82:ARG:NH2   | 2.21                     | 0.73              |
| 49:m3:50:PRO:O     | 49:m3:52:ASP:N     | 2.21                     | 0.73              |
| 3:S1:137:ILE:HD11  | 3:S1:172:LEU:HD22  | 1.69                     | 0.73              |
| 34:SR:89:LEU:HB2   | 34:SR:103:PHE:HB2  | 1.70                     | 0.73              |
| 36:1:3122:A:N1     | 46:L9:70:THR:HG21  | 2.04                     | 0.73              |
| 39:L2:209:HIS:CD2  | 39:L2:211:HIS:H    | 2.06                     | 0.72              |
| 54:M8:154:GLY:O    | 54:M8:159:LYS:HE2  | 1.89                     | 0.72              |
| 1:6:140:A:N6       | 1:6:281:G:OP1      | 2.21                     | 0.72              |
| 36:5:2248:C:OP2    | 86:5:3978:OHX:N6   | 2.22                     | 0.72              |
| 1:2:1181:U:O4      | 86:2:2119:OHX:N6   | 2.23                     | 0.72              |
| 19:C7:14:LYS:NZ    | 19:C7:18:GLU:OE2   | 2.22                     | 0.72              |
| 25:D3:27:ASN:OD1   | 25:D3:31:LYS:NZ    | 2.21                     | 0.72              |
| 41:L4:338:LYS:O    | 41:L4:340:GLY:N    | 2.19                     | 0.72              |
| 45:L8:182:GLY:HA3  | 45:L8:185:ARG:HB2  | 1.70                     | 0.72              |
| 46:l9:28:VAL:HG22  | 46:l9:33:THR:HB    | 1.71                     | 0.72              |
| 59:n3:48:ARG:HH11  | 59:n3:48:ARG:HG3   | 1.53                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:S2:65:GLU:HB2    | 4:S2:68:ILE:HD12   | 1.71                     | 0.72              |
| 36:1:1355:A:H5''   | 36:1:1356:U:H5     | 1.54                     | 0.72              |
| 36:1:1878:G:OP1    | 86:1:3931:OHX:N4   | 2.23                     | 0.72              |
| 36:5:2398:A:H5'    | 36:5:2398:A:C8     | 2.24                     | 0.72              |
| 1:2:7:G:O6         | 4:S2:205:ARG:NH2   | 2.23                     | 0.72              |
| 18:C6:40:GLU:HA    | 18:C6:42:GLU:N     | 2.03                     | 0.72              |
| 36:1:283:G:OP1     | 78:Q2:45:ARG:NH2   | 2.22                     | 0.72              |
| 1:2:452:A:OP2      | 86:2:2039:OHX:N5   | 2.22                     | 0.72              |
| 86:2:2032:OHX:N6   | 86:2:2147:OHX:N5   | 2.36                     | 0.72              |
| 21:C9:49:ASP:HB3   | 21:C9:53:TRP:HB3   | 1.71                     | 0.72              |
| 36:1:439:C:H3'     | 36:1:440:A:C8      | 2.23                     | 0.72              |
| 36:1:1230:G:H1     | 36:1:1279:C:H42    | 1.35                     | 0.72              |
| 28:d6:58:VAL:HG22  | 28:d6:59:TYR:H     | 1.53                     | 0.72              |
| 51:m5:183:THR:OG1  | 51:m5:183:THR:O    | 1.99                     | 0.72              |
| 42:L5:40:HIS:HB3   | 42:L5:43:LYS:HG3   | 1.72                     | 0.72              |
| 44:L7:88:ARG:HD2   | 44:L7:90:LYS:O     | 1.89                     | 0.72              |
| 2:s0:50:VAL:HG23   | 19:c7:109:LEU:HD21 | 1.72                     | 0.72              |
| 40:l3:218:ILE:HG12 | 40:l3:276:THR:HG23 | 1.72                     | 0.72              |
| 52:m6:110:PRO:O    | 52:m6:113:ASP:N    | 2.18                     | 0.72              |
| 52:m6:110:PRO:O    | 52:m6:111:PRO:C    | 2.32                     | 0.72              |
| 60:n4:129:LYS:O    | 60:n4:133:THR:N    | 2.21                     | 0.72              |
| 1:6:542:A:OP1      | 1:6:542:A:H2'      | 1.90                     | 0.72              |
| 41:l4:300:ARG:HG2  | 41:l4:300:ARG:HH11 | 1.53                     | 0.72              |
| 48:m1:82:ARG:NH1   | 48:m1:112:LEU:O    | 2.18                     | 0.72              |
| 62:n6:3:LYS:HD2    | 62:n6:8:VAL:HG23   | 1.71                     | 0.72              |
| 72:o6:54:GLU:HG2   | 72:o6:90:MET:HE1   | 1.72                     | 0.72              |
| 1:2:868:G:H1       | 1:2:960:U:H3       | 1.37                     | 0.72              |
| 24:D2:82:LYS:O     | 24:D2:84:GLY:N     | 2.20                     | 0.72              |
| 27:D5:46:LYS:HG2   | 27:D5:70:LYS:HE3   | 1.72                     | 0.72              |
| 1:6:14:C:OP2       | 4:s2:206:THR:HG21  | 1.89                     | 0.72              |
| 47:m0:38:LYS:HG2   | 47:m0:41:ALA:HB2   | 1.71                     | 0.72              |
| 5:S3:141:LYS:HE3   | 5:S3:179:GLN:HG3   | 1.71                     | 0.72              |
| 15:C3:72:MET:HE1   | 15:C3:82:PRO:HD2   | 1.72                     | 0.72              |
| 12:c0:29:GLN:NE2   | 12:c0:31:LYS:O     | 2.23                     | 0.72              |
| 36:5:364:G:OP1     | 41:l4:60:THR:HG23  | 1.90                     | 0.72              |
| 36:5:2258:U:OP2    | 86:5:3948:OHX:N4   | 2.22                     | 0.72              |
| 36:5:3001:C:OP1    | 40:l3:120:LYS:NZ   | 2.21                     | 0.72              |
| 86:5:3942:OHX:N2   | 86:5:4232:OHX:N6   | 2.38                     | 0.72              |
| 1:2:687:G:H5'      | 24:D2:119:LYS:HG2  | 1.71                     | 0.72              |
| 36:1:3353:G:O2'    | 36:1:3356:G:OP2    | 2.07                     | 0.72              |
| 36:5:1840:U:OP2    | 86:5:4039:OHX:N4   | 2.23                     | 0.72              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:2568:C:N4     | 36:5:2574:G:O6     | 2.23                     | 0.72              |
| 27:D5:65:LEU:HB3   | 27:D5:71:ILE:HD12  | 1.71                     | 0.71              |
| 49:M3:46:ILE:HG23  | 49:M3:49:ARG:HB2   | 1.72                     | 0.71              |
| 63:N7:26:VAL:HG21  | 63:N7:96:VAL:HB    | 1.71                     | 0.71              |
| 70:o4:57:LEU:HB3   | 70:o4:61:GLN:HB2   | 1.72                     | 0.71              |
| 1:2:1207:C:H42     | 1:2:1456:C:H5      | 1.37                     | 0.71              |
| 2:S0:52:LYS:HD2    | 23:D1:82:VAL:HA    | 1.71                     | 0.71              |
| 1:6:1171:A:H2'     | 1:6:1172:G:C8      | 2.25                     | 0.71              |
| 4:S2:245:ASP:N     | 4:S2:245:ASP:OD1   | 2.21                     | 0.71              |
| 36:1:2236:G:OP1    | 86:1:4122:OHX:N6   | 2.23                     | 0.71              |
| 51:M5:96:ARG:HH11  | 51:M5:96:ARG:HG2   | 1.55                     | 0.71              |
| 1:6:1:U:O2'        | 1:6:370:A:H5'      | 1.90                     | 0.71              |
| 40:l3:293:ASN:HB2  | 40:l3:304:THR:HA   | 1.71                     | 0.71              |
| 70:o4:102:LYS:HB3  | 70:o4:103:LYS:HE3  | 1.72                     | 0.71              |
| 3:S1:157:GLN:O     | 3:S1:159:SER:N     | 2.24                     | 0.71              |
| 5:S3:27:ARG:HD2    | 12:C0:60:SER:HB2   | 1.72                     | 0.71              |
| 55:M9:76:SER:O     | 55:M9:81:ARG:NH1   | 2.23                     | 0.71              |
| 1:6:1595:U:N3      | 1:6:1600:A:H2      | 1.87                     | 0.71              |
| 15:c3:65:VAL:HG23  | 15:c3:66:ILE:HG23  | 1.72                     | 0.71              |
| 34:sR:164:ASP:O    | 34:sR:166:SER:N    | 2.23                     | 0.71              |
| 1:2:829:A:O2'      | 1:2:830:U:OP2      | 2.09                     | 0.71              |
| 1:2:1228:G:H1      | 14:C2:67:THR:HB    | 1.54                     | 0.71              |
| 22:D0:48:HIS:ND1   | 22:D0:48:HIS:O     | 2.24                     | 0.71              |
| 36:1:637:C:H2'     | 36:1:638:C:C6      | 2.26                     | 0.71              |
| 36:1:980:A:OP2     | 36:1:980:A:H8      | 1.74                     | 0.71              |
| 49:M3:3:ILE:HG12   | 64:N8:34:MET:HE2   | 1.71                     | 0.71              |
| 2:s0:183:ARG:HG2   | 2:s0:191:ARG:HB3   | 1.72                     | 0.71              |
| 8:s6:31:ARG:HH11   | 8:s6:34:GLN:HE22   | 1.38                     | 0.71              |
| 36:5:2840:C:OP1    | 86:5:4136:OHX:N3   | 2.24                     | 0.71              |
| 16:C4:117:ASP:OD1  | 16:C4:119:THR:HG23 | 1.91                     | 0.71              |
| 21:C9:52:GLY:O     | 21:C9:54:PHE:N     | 2.23                     | 0.71              |
| 36:1:2098:C:H2'    | 36:1:2099:A:H8     | 1.56                     | 0.71              |
| 40:L3:296:THR:HG22 | 40:L3:299:ASP:H    | 1.55                     | 0.71              |
| 4:s2:225:LEU:HD13  | 24:d2:68:ARG:HA    | 1.72                     | 0.71              |
| 25:d3:130:VAL:O    | 25:d3:131:SER:HB3  | 1.89                     | 0.71              |
| 78:q2:71:ARG:HH11  | 78:q2:71:ARG:HG3   | 1.55                     | 0.71              |
| 1:2:1046:G:OP1     | 3:S1:157:GLN:NE2   | 2.23                     | 0.71              |
| 1:2:1585:U:N3      | 1:2:1611:A:H2      | 1.86                     | 0.71              |
| 36:1:3243:A:H4'    | 40:L3:95:THR:HG22  | 1.73                     | 0.71              |
| 40:L3:116:ARG:HG2  | 40:L3:175:LYS:HA   | 1.72                     | 0.71              |
| 42:L5:34:LYS:O     | 42:L5:38:THR:HG23  | 1.89                     | 0.71              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:N6:52:ARG:O    | 62:N6:54:ASP:N     | 2.23                     | 0.71              |
| 51:m5:172:ARG:HB3 | 51:m5:174:ILE:HD13 | 1.72                     | 0.71              |
| 3:S1:48:VAL:HG13  | 3:S1:61:LEU:HD21   | 1.73                     | 0.71              |
| 36:1:2112:U:H4'   | 36:1:2113:A:H5'    | 1.73                     | 0.71              |
| 36:1:2397:A:OP1   | 36:1:2398:A:H4'    | 1.91                     | 0.71              |
| 47:M0:76:MET:HE2  | 47:M0:148:VAL:HG22 | 1.73                     | 0.71              |
| 49:M3:74:GLY:O    | 49:M3:101:ARG:NH1  | 2.24                     | 0.71              |
| 19:c7:51:ALA:O    | 19:c7:55:THR:HG23  | 1.91                     | 0.71              |
| 6:S4:79:ASP:HB3   | 6:S4:82:TYR:HB2    | 1.72                     | 0.71              |
| 18:c6:39:VAL:HG12 | 18:c6:41:PRO:HD2   | 1.73                     | 0.71              |
| 41:l4:302:ALA:HB2 | 54:m8:39:ARG:CZ    | 2.21                     | 0.71              |
| 1:2:887:A:H1'     | 16:C4:122:PRO:HB3  | 1.73                     | 0.71              |
| 6:S4:158:ASP:OD2  | 6:S4:174:LYS:NZ    | 2.23                     | 0.71              |
| 16:C4:50:ALA:O    | 16:C4:52:ARG:N     | 2.24                     | 0.71              |
| 41:L4:181:VAL:O   | 41:L4:182:LEU:HB2  | 1.91                     | 0.71              |
| 1:6:1370:U:H4'    | 1:6:1371:A:H4'     | 1.73                     | 0.71              |
| 14:c2:28:LEU:HD11 | 14:c2:89:ILE:HG21  | 1.71                     | 0.71              |
| 1:2:218:A:O2'     | 1:2:219:A:OP1      | 2.08                     | 0.70              |
| 1:2:1657:U:H4'    | 1:2:1658:G:O5'     | 1.89                     | 0.70              |
| 36:1:1238:C:N4    | 36:1:1245:A:OP2    | 2.20                     | 0.70              |
| 1:6:1098:U:OP2    | 4:s2:168:ARG:NE    | 2.23                     | 0.70              |
| 7:s5:222:LYS:HA   | 7:s5:225:ARG:HH11  | 1.53                     | 0.70              |
| 18:c6:82:ARG:HH22 | 18:c6:114:ARG:HG3  | 1.55                     | 0.70              |
| 1:2:656:G:O2'     | 1:2:657:U:O4'      | 2.08                     | 0.70              |
| 36:1:595:G:N1     | 36:1:609:G:H5''    | 2.06                     | 0.70              |
| 36:1:1952:G:H3'   | 36:1:1953:G:H5''   | 1.73                     | 0.70              |
| 36:1:2734:A:OP1   | 86:1:4010:OHX:N3   | 2.24                     | 0.70              |
| 17:c5:44:ARG:NH2  | 17:c5:82:ASN:O     | 2.23                     | 0.70              |
| 38:8:41:A:O2'     | 73:o7:59:THR:HG22  | 1.90                     | 0.70              |
| 62:n6:112:ASP:HB3 | 62:n6:115:ARG:HB2  | 1.73                     | 0.70              |
| 9:S7:50:ASP:OD1   | 9:S7:50:ASP:N      | 2.23                     | 0.70              |
| 36:1:3312:U:H5''  | 40:L3:25:ILE:HD12  | 1.73                     | 0.70              |
| 4:s2:90:THR:O     | 4:s2:92:ALA:N      | 2.22                     | 0.70              |
| 16:c4:86:THR:HB   | 16:c4:91:THR:HG22  | 1.73                     | 0.70              |
| 19:C7:82:ASP:O    | 19:C7:83:GLN:NE2   | 2.21                     | 0.70              |
| 33:E1:127:GLY:O   | 33:E1:129:GLY:N    | 2.24                     | 0.70              |
| 36:1:299:G:N7     | 86:1:4084:OHX:N2   | 2.39                     | 0.70              |
| 48:M1:49:LYS:HB3  | 48:M1:62:ASN:HA    | 1.73                     | 0.70              |
| 63:N7:70:PRO:HG3  | 63:N7:115:LYS:HB2  | 1.73                     | 0.70              |
| 21:c9:37:VAL:HG11 | 21:c9:100:ILE:HD11 | 1.74                     | 0.70              |
| 36:5:3107:U:OP1   | 76:q0:114:LYS:NZ   | 2.24                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:5:3942:OHX:N2   | 86:5:4232:OHX:N4   | 2.38                     | 0.70              |
| 41:14:59:GLN:OE1   | 73:o7:55:ARG:NH2   | 2.24                     | 0.70              |
| 17:C5:39:ALA:HA    | 17:C5:42:ARG:HH21  | 1.55                     | 0.70              |
| 59:N3:87:ARG:HH22  | 59:N3:137:VAL:CG2  | 2.05                     | 0.70              |
| 68:O2:81:ASP:O     | 68:O2:84:THR:HG23  | 1.90                     | 0.70              |
| 1:6:193:U:C2       | 1:6:195:G:H1'      | 2.26                     | 0.70              |
| 1:6:1492:A:O2'     | 1:6:1493:A:H8      | 1.75                     | 0.70              |
| 1:6:1670:G:N7      | 86:6:2190:OHX:N4   | 2.38                     | 0.70              |
| 10:s8:57:ALA:HB2   | 10:s8:177:GLY:HA2  | 1.74                     | 0.70              |
| 41:14:36:HIS:O     | 41:14:40:THR:HG23  | 1.92                     | 0.70              |
| 56:n0:137:ARG:HG2  | 56:n0:139:TYR:CE1  | 2.26                     | 0.70              |
| 1:2:833:U:OP2      | 86:2:2142:OHX:N4   | 2.25                     | 0.70              |
| 1:2:1428:G:H5'     | 1:2:1428:G:H8      | 1.56                     | 0.70              |
| 1:2:1796:C:H5      | 28:D6:6:ALA:H      | 1.39                     | 0.70              |
| 36:1:3298:C:OP1    | 53:M7:74:LYS:NZ    | 2.23                     | 0.70              |
| 1:6:25:C:OP2       | 1:6:25:C:H4'       | 1.90                     | 0.70              |
| 1:6:176:C:OP1      | 86:6:2096:OHX:N6   | 2.25                     | 0.70              |
| 1:6:1542:G:N2      | 1:6:1569:A:OP2     | 2.25                     | 0.70              |
| 36:5:283:G:OP1     | 78:q2:45:ARG:NH2   | 2.22                     | 0.70              |
| 36:5:2123:G:N7     | 86:5:4099:OHX:N1   | 2.39                     | 0.70              |
| 47:m0:174:THR:OG1  | 47:m0:175:ASN:O    | 2.05                     | 0.70              |
| 1:2:150:U:OP1      | 26:D4:123:LYS:NZ   | 2.24                     | 0.70              |
| 36:1:980:A:H2'     | 36:1:981:U:N1      | 2.06                     | 0.70              |
| 1:6:397:A:O3'      | 10:s8:50:GLY:HA2   | 1.92                     | 0.70              |
| 17:c5:111:MET:HG2  | 20:c8:119:ILE:HG13 | 1.72                     | 0.70              |
| 36:5:770:G:N7      | 86:5:4096:OHX:N6   | 2.39                     | 0.70              |
| 40:l3:239:PRO:O    | 40:l3:242:THR:HG23 | 1.90                     | 0.70              |
| 86:2:2090:OHX:N6   | 77:Q1:25:LYS:O     | 2.24                     | 0.70              |
| 36:1:1790:G:O6     | 86:1:4171:OHX:N4   | 2.25                     | 0.70              |
| 54:M8:30:VAL:O     | 54:M8:34:THR:HG23  | 1.91                     | 0.70              |
| 1:6:1202:A:OP1     | 86:6:2130:OHX:N2   | 2.24                     | 0.70              |
| 10:s8:138:ASN:HA   | 10:s8:141:ARG:HD3  | 1.74                     | 0.70              |
| 36:5:979:U:H1'     | 36:5:980:A:C4      | 2.26                     | 0.70              |
| 2:S0:71:GLU:O      | 2:S0:96:THR:HG22   | 1.91                     | 0.70              |
| 5:s3:225:TYR:OH    | 34:sR:191:ASP:OD2  | 2.10                     | 0.70              |
| 6:s4:19:LEU:HD11   | 6:s4:108:ARG:HD2   | 1.71                     | 0.70              |
| 64:n8:104:THR:HG21 | 64:n8:112:ILE:HD11 | 1.73                     | 0.70              |
| 9:S7:38:LEU:HD23   | 9:S7:41:LEU:HD12   | 1.73                     | 0.70              |
| 36:1:2107:A:H2     | 36:1:3344:A:H8     | 1.39                     | 0.70              |
| 45:l8:78:PHE:O     | 45:l8:79:GLN:HB3   | 1.91                     | 0.70              |
| 1:2:1199:G:O6      | 22:D0:67:THR:HG23  | 1.92                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:C2:66:VAL:HG11  | 14:C2:71:ILE:HD12  | 1.74                     | 0.69              |
| 36:1:2736:A:O2'    | 57:N1:68:THR:HG21  | 1.92                     | 0.69              |
| 36:1:2818:U:H6     | 36:1:2818:U:H5'    | 1.56                     | 0.69              |
| 46:L9:48:VAL:HG11  | 46:L9:52:LEU:HD13  | 1.74                     | 0.69              |
| 1:6:67:A:O2'       | 1:6:69:G:OP1       | 2.06                     | 0.69              |
| 10:s8:8:ARG:HH21   | 10:s8:22:ARG:HH11  | 1.37                     | 0.69              |
| 14:c2:61:VAL:HG13  | 14:c2:121:VAL:HG23 | 1.74                     | 0.69              |
| 1:2:1460:A:OP2     | 35:SM:68:ARG:HD3   | 1.91                     | 0.69              |
| 86:2:2032:OHX:N3   | 86:2:2147:OHX:N1   | 2.40                     | 0.69              |
| 2:S0:49:ASN:HB3    | 2:S0:52:LYS:HG3    | 1.74                     | 0.69              |
| 1:2:513:U:H2'      | 1:2:514:G:C8       | 2.27                     | 0.69              |
| 1:2:885:G:OP1      | 3:S1:136:ARG:NH1   | 2.25                     | 0.69              |
| 1:2:1537:C:N3      | 86:2:2155:OHX:N3   | 2.39                     | 0.69              |
| 7:S5:123:VAL:O     | 27:D5:58:ARG:NH1   | 2.24                     | 0.69              |
| 36:1:1495:U:H5     | 36:1:1835:A:N1     | 1.91                     | 0.69              |
| 36:1:2120:A:OP2    | 86:1:4012:OHX:N2   | 2.25                     | 0.69              |
| 41:L4:269:SER:O    | 41:L4:271:LYS:N    | 2.22                     | 0.69              |
| 35:sM:65:THR:OG1   | 35:sM:66:ALA:N     | 2.23                     | 0.69              |
| 42:l5:270:LYS:HG3  | 42:l5:273:ARG:CB   | 2.23                     | 0.69              |
| 9:S7:13:PRO:HB3    | 9:S7:14:THR:HB     | 1.73                     | 0.69              |
| 17:C5:69:GLU:OE1   | 86:C5:201:OHX:N4   | 2.25                     | 0.69              |
| 36:1:364:G:OP1     | 41:L4:60:THR:HG23  | 1.92                     | 0.69              |
| 38:4:106:C:O2'     | 86:4:232:OHX:N4    | 2.25                     | 0.69              |
| 41:L4:354:VAL:O    | 41:L4:358:THR:HG23 | 1.92                     | 0.69              |
| 42:L5:294:ALA:HB1  | 47:M0:217:PHE:HB3  | 1.73                     | 0.69              |
| 72:O6:76:ARG:HA    | 72:O6:76:ARG:HE    | 1.57                     | 0.69              |
| 1:6:1796:C:OP1     | 28:d6:87:ARG:NH1   | 2.24                     | 0.69              |
| 19:c7:105:GLN:HA   | 19:c7:108:ASP:HB2  | 1.74                     | 0.69              |
| 34:sR:89:LEU:HB2   | 34:sR:103:PHE:HB2  | 1.73                     | 0.69              |
| 36:5:2101:C:O2'    | 36:5:2102:U:OP1    | 2.10                     | 0.69              |
| 45:l8:160:ILE:HD12 | 45:l8:164:VAL:HG13 | 1.75                     | 0.69              |
| 1:2:134:U:OP1      | 1:2:136:C:N4       | 2.25                     | 0.69              |
| 1:2:176:C:OP1      | 86:2:2074:OHX:N3   | 2.25                     | 0.69              |
| 36:1:3107:U:OP1    | 76:Q0:114:LYS:NZ   | 2.25                     | 0.69              |
| 37:3:62:U:O3'      | 42:L5:285:ARG:NH1  | 2.25                     | 0.69              |
| 53:M7:29:THR:HG22  | 53:M7:87:SER:OG    | 1.92                     | 0.69              |
| 68:O2:91:THR:HG22  | 68:O2:92:TYR:HD2   | 1.56                     | 0.69              |
| 3:s1:169:SER:O     | 3:s1:173:THR:HG23  | 1.93                     | 0.69              |
| 20:c8:30:TYR:O     | 20:c8:33:THR:OG1   | 2.10                     | 0.69              |
| 36:5:2836:C:H5     | 36:5:2852:C:N4     | 1.90                     | 0.69              |
| 36:5:2970:C:H4'    | 36:5:2971:A:N1     | 2.07                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:8:53:A:OP1      | 75:o9:19:GLN:NE2   | 2.25                     | 0.69              |
| 51:m5:183:THR:HG22 | 51:m5:187:ARG:HB2  | 1.74                     | 0.69              |
| 1:2:1592:A:H2'     | 1:2:1593:A:H8      | 1.58                     | 0.69              |
| 36:1:1409:G:N7     | 86:1:4070:OHX:N3   | 2.41                     | 0.69              |
| 46:L9:17:THR:HG21  | 50:M4:3:THR:HB     | 1.73                     | 0.69              |
| 62:N6:45:ILE:HD11  | 62:N6:122:LYS:HB2  | 1.75                     | 0.69              |
| 4:s2:139:ILE:HD11  | 4:s2:191:ALA:HB1   | 1.74                     | 0.69              |
| 31:d9:33:LYS:HE2   | 31:d9:34:TYR:CZ    | 2.28                     | 0.69              |
| 36:5:1772:U:H5''   | 36:5:1773:C:H5'    | 1.74                     | 0.69              |
| 56:n0:155:ARG:HD3  | 56:n0:172:TYR:CG   | 2.28                     | 0.69              |
| 71:o5:76:GLN:O     | 71:o5:81:ARG:NH1   | 2.26                     | 0.69              |
| 1:2:732:G:O2'      | 1:2:733:A:O4'      | 2.10                     | 0.69              |
| 46:L9:171:ASP:OD1  | 46:L9:173:ARG:HD3  | 1.93                     | 0.69              |
| 13:c1:33:ARG:NH2   | 13:c1:51:GLY:O     | 2.25                     | 0.69              |
| 36:5:1875:G:C2'    | 36:5:1876:U:H5''   | 2.23                     | 0.69              |
| 1:2:759:U:OP1      | 86:2:2161:OHX:N1   | 2.26                     | 0.69              |
| 1:2:1533:C:H4'     | 1:2:1539:G:N1      | 2.08                     | 0.69              |
| 18:C6:32:ASN:O     | 18:C6:66:ARG:NH1   | 2.25                     | 0.69              |
| 36:1:1493:G:O6     | 75:O9:2:ALA:HA     | 1.93                     | 0.69              |
| 36:1:2307:G:O2'    | 36:1:2310:U:OP2    | 2.10                     | 0.69              |
| 36:1:2585:G:N7     | 45:L8:47:SER:OG    | 2.25                     | 0.69              |
| 47:M0:3:ARG:NH1    | 47:M0:63:GLU:HG3   | 2.07                     | 0.69              |
| 1:6:330:G:OP2      | 10:s8:172:ARG:NH1  | 2.26                     | 0.69              |
| 36:5:200:C:OP1     | 62:n6:60:ARG:NH1   | 2.25                     | 0.69              |
| 36:5:3295:A:H2'    | 36:5:3296:A:C8     | 2.27                     | 0.69              |
| 47:m0:38:LYS:NZ    | 47:m0:45:GLU:OE2   | 2.25                     | 0.69              |
| 73:o7:21:ARG:NH2   | 73:o7:41:ALA:O     | 2.26                     | 0.69              |
| 4:S2:116:LYS:HG2   | 4:S2:127:ALA:HB3   | 1.74                     | 0.69              |
| 19:C7:34:LEU:O     | 19:C7:38:ILE:HG22  | 1.93                     | 0.69              |
| 40:L3:239:PRO:O    | 40:L3:242:THR:HG23 | 1.92                     | 0.69              |
| 41:L4:47:ARG:NH1   | 41:L4:109:TRP:O    | 2.25                     | 0.69              |
| 55:M9:105:LEU:HD23 | 55:M9:138:LEU:HD13 | 1.75                     | 0.69              |
| 57:N1:39:ILE:HD12  | 57:N1:102:ARG:HG2  | 1.74                     | 0.69              |
| 34:sR:184:ASN:HD22 | 34:sR:185:GLN:N    | 1.91                     | 0.69              |
| 36:5:2211:U:O4     | 86:5:3962:OHX:N4   | 2.26                     | 0.69              |
| 48:m1:168:ASP:OD1  | 86:m1:203:OHX:N3   | 2.26                     | 0.69              |
| 63:n7:135:ARG:HB3  | 63:n7:135:ARG:HH21 | 1.57                     | 0.69              |
| 24:D2:76:SER:OG    | 24:D2:77:PRO:HD3   | 1.93                     | 0.69              |
| 36:1:3358:U:H2'    | 36:1:3359:A:O4'    | 1.93                     | 0.69              |
| 1:6:915:A:OP1      | 86:6:2071:OHX:N6   | 2.26                     | 0.69              |
| 34:sR:52:GLN:HG2   | 34:sR:53:LYS:H     | 1.58                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1804:A:H2'    | 36:5:1805:C:C6     | 2.28                     | 0.69              |
| 1:2:1726:G:N7      | 86:2:2099:OHX:N4   | 2.41                     | 0.68              |
| 11:S9:109:LEU:HB2  | 11:S9:146:PHE:HB3  | 1.75                     | 0.68              |
| 11:S9:110:GLN:HE22 | 11:S9:126:ARG:HG2  | 1.58                     | 0.68              |
| 15:C3:132:VAL:HG23 | 15:C3:134:VAL:HG13 | 1.74                     | 0.68              |
| 36:1:824:C:H5''    | 39:L2:21:ARG:HD3   | 1.76                     | 0.68              |
| 38:4:136:G:OP1     | 61:N5:48:SER:OG    | 2.11                     | 0.68              |
| 39:L2:114:SER:HB2  | 39:L2:169:ILE:HD12 | 1.75                     | 0.68              |
| 1:6:578:U:H4'      | 1:6:579:A:H5'      | 1.75                     | 0.68              |
| 8:s6:67:VAL:HG23   | 8:s6:68:LEU:O      | 1.93                     | 0.68              |
| 15:c3:25:TRP:HA    | 15:c3:27:LYS:HE2   | 1.75                     | 0.68              |
| 18:c6:49:TYR:HB3   | 18:c6:53:LEU:HD21  | 1.74                     | 0.68              |
| 42:l5:95:TRP:CH2   | 42:l5:181:PRO:HD3  | 2.28                     | 0.68              |
| 1:2:61:A:H8        | 1:2:269:G:HO2'     | 1.39                     | 0.68              |
| 36:1:3087:A:OP1    | 86:1:4184:OHX:N5   | 2.26                     | 0.68              |
| 86:1:3876:OHX:N5   | 38:4:2:A:OP2       | 2.26                     | 0.68              |
| 1:6:1769:U:OP2     | 86:6:2144:OHX:N2   | 2.26                     | 0.68              |
| 10:s8:120:THR:O    | 86:s8:303:OHX:N4   | 2.25                     | 0.68              |
| 45:l8:94:PHE:HB3   | 45:l8:189:LEU:HD11 | 1.74                     | 0.68              |
| 1:6:320:U:H2'      | 1:6:321:C:C2       | 2.28                     | 0.68              |
| 47:m0:87:LEU:HD23  | 47:m0:138:VAL:HG22 | 1.75                     | 0.68              |
| 66:o0:9:SER:OG     | 66:o0:10:ILE:N     | 2.26                     | 0.68              |
| 7:S5:92:ARG:NH2    | 7:S5:169:ASN:OD1   | 2.26                     | 0.68              |
| 36:1:1320:C:O2     | 56:N0:115:ARG:NH2  | 2.25                     | 0.68              |
| 1:6:1402:G:OP2     | 19:c7:5:ARG:NH1    | 2.26                     | 0.68              |
| 36:5:1387:G:OP1    | 86:5:4198:OHX:N3   | 2.27                     | 0.68              |
| 37:7:5:G:OP1       | 48:m1:143:ARG:NH2  | 2.26                     | 0.68              |
| 1:2:377:G:O6       | 86:2:2079:OHX:N5   | 2.25                     | 0.68              |
| 2:S0:24:LEU:O      | 2:S0:163:ASN:ND2   | 2.27                     | 0.68              |
| 3:S1:34:ALA:HB3    | 3:S1:41:ARG:HA     | 1.76                     | 0.68              |
| 36:1:978:G:O2'     | 36:1:979:U:O2      | 2.11                     | 0.68              |
| 36:1:2854:U:OP2    | 47:M0:3:ARG:NH2    | 2.27                     | 0.68              |
| 86:1:4084:OHX:N1   | 72:O6:28:TYR:O     | 2.26                     | 0.68              |
| 53:M7:29:THR:HA    | 53:M7:32:THR:HG23  | 1.75                     | 0.68              |
| 66:O0:13:LYS:NZ    | 66:O0:99:ASP:OD2   | 2.26                     | 0.68              |
| 1:6:822:U:H2'      | 1:6:823:G:H5''     | 1.76                     | 0.68              |
| 1:6:1619:C:C2      | 30:d8:22:ARG:HD2   | 2.29                     | 0.68              |
| 19:c7:103:ASP:O    | 19:c7:104:ASN:ND2  | 2.25                     | 0.68              |
| 33:e1:144:CYS:HB3  | 33:e1:147:VAL:HG13 | 1.74                     | 0.68              |
| 36:5:1095:U:H3     | 57:n1:127:GLN:HG3  | 1.59                     | 0.68              |
| 37:7:1:G:N3        | 42:l5:269:SER:OG   | 2.23                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:l4:354:VAL:O    | 41:l4:358:THR:HG23 | 1.92                     | 0.68              |
| 53:m7:125:GLN:HB2  | 53:m7:141:SER:HB2  | 1.74                     | 0.68              |
| 18:C6:58:ASP:O     | 18:C6:60:PHE:N     | 2.25                     | 0.68              |
| 36:1:2548:C:OP2    | 39:L2:93:LYS:NZ    | 2.25                     | 0.68              |
| 1:6:1597:A:OP1     | 31:d9:19:ARG:NH2   | 2.23                     | 0.68              |
| 9:s7:114:ARG:O     | 9:s7:117:THR:HB    | 1.94                     | 0.68              |
| 36:5:2682:C:OP2    | 48:m1:51:ARG:NH2   | 2.27                     | 0.68              |
| 3:S1:70:LEU:O      | 3:S1:74:GLN:N      | 2.26                     | 0.68              |
| 8:S6:102:VAL:HG13  | 8:S6:106:LEU:HD12  | 1.75                     | 0.68              |
| 36:1:2924:U:O4     | 86:1:4021:OHX:N1   | 2.26                     | 0.68              |
| 1:2:1595:U:H3      | 1:2:1600:A:H2      | 1.42                     | 0.68              |
| 18:C6:143:ARG:HH12 | 35:SM:84:LYS:HZ3   | 1.40                     | 0.68              |
| 20:C8:123:ARG:HG3  | 20:C8:133:VAL:HG21 | 1.76                     | 0.68              |
| 47:M0:36:LEU:HD21  | 47:M0:69:ARG:HH11  | 1.58                     | 0.68              |
| 76:Q0:92:ASP:O     | 76:Q0:105:PRO:HG3  | 1.94                     | 0.68              |
| 36:5:1677:G:OP2    | 58:n2:103:TYR:OH   | 2.08                     | 0.68              |
| 57:n1:139:ARG:HG2  | 57:n1:139:ARG:HH21 | 1.59                     | 0.68              |
| 61:n5:51:VAL:HG21  | 71:o5:62:GLN:HB3   | 1.75                     | 0.68              |
| 64:n8:3:SER:O      | 64:n8:6:THR:HB     | 1.93                     | 0.68              |
| 64:n8:28:HIS:CD2   | 64:n8:32:ARG:HG2   | 2.28                     | 0.68              |
| 1:2:68:A:H5'       | 8:S6:160:ARG:HH12  | 1.59                     | 0.68              |
| 36:1:368:G:OP1     | 86:1:3887:OHX:N1   | 2.27                     | 0.68              |
| 36:1:541:U:O4      | 86:1:4196:OHX:N2   | 2.27                     | 0.68              |
| 38:4:97:A:OP1      | 71:O5:67:ARG:NH2   | 2.26                     | 0.68              |
| 59:N3:87:ARG:HH22  | 59:N3:137:VAL:HG21 | 1.59                     | 0.68              |
| 36:5:1110:U:H2'    | 36:5:1111:U:C6     | 2.29                     | 0.68              |
| 36:5:1364:C:OP1    | 44:l7:110:ARG:NH2  | 2.26                     | 0.68              |
| 54:m8:153:PHE:O    | 54:m8:161:LYS:HG2  | 1.93                     | 0.68              |
| 1:2:151:G:O6       | 26:D4:124:ARG:NH2  | 2.25                     | 0.68              |
| 9:S7:50:ASP:HB3    | 9:S7:56:LYS:HG2    | 1.76                     | 0.68              |
| 1:6:513:U:H2'      | 1:6:514:G:C8       | 2.29                     | 0.68              |
| 34:sR:7:LEU:HG     | 34:sR:315:VAL:HG22 | 1.75                     | 0.68              |
| 86:5:3978:OHX:N2   | 86:5:4196:OHX:N1   | 2.41                     | 0.68              |
| 45:l8:33:ASN:O     | 45:l8:35:GLY:N     | 2.27                     | 0.68              |
| 58:n2:19:VAL:O     | 58:n2:23:THR:OG1   | 2.11                     | 0.68              |
| 1:2:514:G:H1       | 1:2:543:C:H5       | 1.42                     | 0.67              |
| 2:S0:74:VAL:HG22   | 2:S0:96:THR:HG23   | 1.76                     | 0.67              |
| 1:6:895:G:H1       | 1:6:917:U:H3       | 1.41                     | 0.67              |
| 86:6:2121:OHX:N6   | 86:6:2171:OHX:N3   | 2.42                     | 0.67              |
| 36:5:600:G:N2      | 36:5:603:A:OP2     | 2.28                     | 0.67              |
| 36:5:1688:U:H2'    | 36:5:1689:U:C6     | 2.29                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1806:A:OP2    | 86:5:4024:OHX:N5   | 2.27                     | 0.67              |
| 20:C8:120:ARG:NH2  | 35:SM:58:GLU:OE1   | 2.26                     | 0.67              |
| 36:1:1078:U:O4     | 86:1:3970:OHX:N2   | 2.28                     | 0.67              |
| 36:1:1794:G:H4'    | 39:L2:191:LEU:HD13 | 1.74                     | 0.67              |
| 1:6:1533:C:H4'     | 1:6:1539:G:N1      | 2.08                     | 0.67              |
| 33:e1:119:ARG:NH2  | 33:e1:120:GLU:O    | 2.27                     | 0.67              |
| 36:5:155:G:H5''    | 36:5:156:G:C8      | 2.29                     | 0.67              |
| 36:5:2877:G:OP1    | 86:5:4054:OHX:N4   | 2.28                     | 0.67              |
| 1:2:66:U:H5        | 8:S6:173:PRO:HG3   | 1.59                     | 0.67              |
| 46:L9:9:GLN:HG2    | 46:L9:52:LEU:HD21  | 1.75                     | 0.67              |
| 49:M3:122:LYS:NZ   | 71:O5:119:LYS:O    | 2.26                     | 0.67              |
| 5:s3:211:PRO:HG2   | 19:c7:19:ARG:HB2   | 1.76                     | 0.67              |
| 7:s5:36:ALA:HB1    | 7:s5:42:LEU:HD12   | 1.75                     | 0.67              |
| 12:c0:32:HIS:CD2   | 12:c0:33:GLU:H     | 2.12                     | 0.67              |
| 13:c1:18:HIS:O     | 86:c1:202:OHX:N3   | 2.27                     | 0.67              |
| 36:5:118:U:O2      | 36:5:121:A:H5'     | 1.93                     | 0.67              |
| 70:o4:7:PHE:CD1    | 70:o4:20:ILE:HD12  | 2.30                     | 0.67              |
| 1:2:197:A:H61      | 10:S8:138:ASN:ND2  | 1.92                     | 0.67              |
| 1:2:1680:G:O6      | 86:2:2110:OHX:N5   | 2.27                     | 0.67              |
| 36:1:103:G:OP1     | 49:M3:70:ARG:NH2   | 2.26                     | 0.67              |
| 36:1:3316:A:O2'    | 36:1:3317:U:OP2    | 2.08                     | 0.67              |
| 47:M0:14:ASN:O     | 47:M0:128:ARG:NH2  | 2.28                     | 0.67              |
| 63:N7:38:PHE:O     | 63:N7:40:HIS:ND1   | 2.23                     | 0.67              |
| 20:c8:134:ARG:O    | 20:c8:136:GLN:NE2  | 2.27                     | 0.67              |
| 22:d0:71:PRO:O     | 22:d0:72:ASN:ND2   | 2.27                     | 0.67              |
| 5:S3:164:VAL:HG13  | 5:S3:168:ILE:HD11  | 1.76                     | 0.67              |
| 86:1:3943:OHX:N5   | 86:1:4200:OHX:N6   | 2.42                     | 0.67              |
| 51:M5:15:GLN:HB3   | 72:O6:51:SER:HB2   | 1.76                     | 0.67              |
| 54:M8:64:VAL:HG22  | 54:M8:96:PHE:CE2   | 2.29                     | 0.67              |
| 64:N8:96:LYS:O     | 64:N8:98:THR:N     | 2.27                     | 0.67              |
| 1:6:1492:A:HO2'    | 1:6:1493:A:H8      | 1.42                     | 0.67              |
| 9:s7:67:LEU:HG     | 9:s7:94:ALA:HB2    | 1.75                     | 0.67              |
| 11:s9:110:GLN:HE22 | 11:s9:126:ARG:HG2  | 1.59                     | 0.67              |
| 13:c1:101:GLU:OE2  | 25:d3:16:ARG:NH2   | 2.27                     | 0.67              |
| 17:c5:65:LEU:O     | 86:c5:201:OHX:N2   | 2.28                     | 0.67              |
| 20:c8:30:TYR:HE2   | 20:c8:40:ARG:HH11  | 1.42                     | 0.67              |
| 29:d7:56:CYS:SG    | 29:d7:57:GLU:N     | 2.67                     | 0.67              |
| 86:7:218:OHX:N3    | 86:7:226:OHX:N6    | 2.43                     | 0.67              |
| 43:l6:149:ILE:HG23 | 43:l6:155:LEU:HD13 | 1.75                     | 0.67              |
| 1:2:523:G:OP2      | 26:D4:37:LYS:NZ    | 2.20                     | 0.67              |
| 22:D0:106:ILE:HG23 | 22:D0:107:THR:HG23 | 1.77                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 65:N9:14:ARG:HH22 | 65:N9:18:ARG:HH11  | 1.42                     | 0.67              |
| 76:Q0:77:ILE:HG22 | 76:Q0:78:ILE:H     | 1.59                     | 0.67              |
| 78:Q2:77:CYS:SG   | 78:Q2:79:THR:HG23  | 2.35                     | 0.67              |
| 1:6:1590:G:OP2    | 86:6:2157:OHX:N6   | 2.27                     | 0.67              |
| 86:6:2121:OHX:N6  | 86:6:2171:OHX:N5   | 2.43                     | 0.67              |
| 11:s9:171:ARG:NH1 | 11:s9:174:ARG:HD3  | 2.10                     | 0.67              |
| 36:5:343:U:OP2    | 86:5:3924:OHX:N3   | 2.28                     | 0.67              |
| 36:5:1466:G:O6    | 86:5:3912:OHX:N5   | 2.28                     | 0.67              |
| 36:5:2586:G:N7    | 45:l8:241:LYS:HB2  | 2.09                     | 0.67              |
| 45:l8:81:THR:OG1  | 45:l8:82:LEU:N     | 2.19                     | 0.67              |
| 5:S3:211:PRO:HG2  | 19:C7:19:ARG:HB2   | 1.75                     | 0.67              |
| 36:1:223:U:O4     | 86:1:4198:OHX:N5   | 2.27                     | 0.67              |
| 38:4:52:A:H62     | 75:O9:27:ILE:HD13  | 1.59                     | 0.67              |
| 61:N5:38:LEU:HD11 | 61:N5:40:LEU:HD13  | 1.77                     | 0.67              |
| 75:O9:50:ASN:OD1  | 86:O9:101:OHX:N6   | 2.28                     | 0.67              |
| 1:6:647:G:H22     | 1:6:687:G:H22      | 1.41                     | 0.67              |
| 42:l5:296:GLN:HG2 | 47:m0:214:PRO:HB3  | 1.76                     | 0.67              |
| 49:m3:56:PRO:HG3  | 49:m3:74:GLY:O     | 1.94                     | 0.67              |
| 1:2:915:A:OP1     | 86:2:2095:OHX:N3   | 2.27                     | 0.67              |
| 9:S7:50:ASP:HA    | 9:S7:56:LYS:HA     | 1.77                     | 0.67              |
| 26:D4:47:VAL:O    | 26:D4:49:LYS:NZ    | 2.21                     | 0.67              |
| 4:s2:163:GLY:O    | 4:s2:164:SER:HB3   | 1.94                     | 0.67              |
| 5:s3:125:TYR:O    | 5:s3:129:SER:OG    | 2.12                     | 0.67              |
| 5:s3:222:VAL:HG11 | 34:sR:229:LYS:HA   | 1.75                     | 0.67              |
| 8:s6:71:THR:HG22  | 8:s6:72:ARG:H      | 1.58                     | 0.67              |
| 26:d4:20:ARG:HE   | 26:d4:22:GLN:HE21  | 1.42                     | 0.67              |
| 36:5:92:G:H5'     | 36:5:93:C:H5''     | 1.76                     | 0.67              |
| 36:5:1098:A:O5'   | 57:n1:129:LYS:HB2  | 1.95                     | 0.67              |
| 42:l5:105:ILE:O   | 42:l5:109:THR:HG23 | 1.94                     | 0.67              |
| 57:n1:42:ILE:HG12 | 57:n1:96:ILE:HD11  | 1.77                     | 0.67              |
| 1:2:1745:G:O6     | 86:2:2087:OHX:N6   | 2.28                     | 0.67              |
| 4:S2:178:ILE:O    | 4:S2:185:LYS:NZ    | 2.21                     | 0.67              |
| 25:D3:79:ASN:HB3  | 25:D3:81:LYS:H     | 1.58                     | 0.67              |
| 36:1:1752:A:OP2   | 86:1:4051:OHX:N3   | 2.28                     | 0.67              |
| 38:4:95:G:OP2     | 73:O7:72:ARG:NH1   | 2.27                     | 0.67              |
| 42:l5:265:TYR:O   | 42:l5:269:SER:HB3  | 1.95                     | 0.67              |
| 1:6:729:G:O2'     | 1:6:730:G:O5'      | 2.12                     | 0.67              |
| 1:6:1762:A:H1'    | 1:6:1783:C:H5'     | 1.77                     | 0.67              |
| 1:2:178:U:C4      | 8:S6:191:ARG:HD3   | 2.30                     | 0.66              |
| 31:D9:19:ARG:HD2  | 31:D9:32:ARG:HD2   | 1.76                     | 0.66              |
| 42:L5:294:ALA:O   | 42:L5:296:GLN:N    | 2.23                     | 0.66              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:M5:150:TRP:CH2 | 51:M5:151:ILE:HG12 | 2.29                     | 0.66              |
| 1:6:66:U:OP1      | 8:s6:136:LYS:NZ    | 2.20                     | 0.66              |
| 1:6:868:G:H1      | 1:6:960:U:H3       | 1.42                     | 0.66              |
| 40:l3:41:VAL:HA   | 40:l3:185:GLY:CA   | 2.23                     | 0.66              |
| 51:m5:190:THR:O   | 51:m5:194:GLN:HG2  | 1.94                     | 0.66              |
| 1:2:1202:A:N6     | 1:2:1457:C:H5''    | 2.11                     | 0.66              |
| 2:S0:31:VAL:HG12  | 2:S0:33:GLN:H      | 1.60                     | 0.66              |
| 47:M0:171:TRP:O   | 47:M0:174:THR:HB   | 1.95                     | 0.66              |
| 20:c8:13:HIS:HA   | 20:c8:24:GLY:HA3   | 1.76                     | 0.66              |
| 22:d0:58:LEU:HD13 | 22:d0:88:LYS:HE3   | 1.76                     | 0.66              |
| 29:d7:37:CYS:O    | 29:d7:39:GLY:N     | 2.19                     | 0.66              |
| 36:5:398:A:O2'    | 36:5:1416:C:OP1    | 2.11                     | 0.66              |
| 44:l7:151:ARG:NH1 | 44:l7:244:ASN:O    | 2.29                     | 0.66              |
| 36:1:1636:U:H5''  | 63:N7:73:LYS:NZ    | 2.10                     | 0.66              |
| 1:6:1280:C:H2'    | 1:6:1281:G:C8      | 2.31                     | 0.66              |
| 20:c8:28:ILE:HD11 | 20:c8:56:LYS:HB2   | 1.77                     | 0.66              |
| 36:5:15:C:H6      | 36:5:15:C:H5'      | 1.59                     | 0.66              |
| 43:l6:50:LYS:HG2  | 43:l6:74:VAL:HG21  | 1.77                     | 0.66              |
| 1:2:1683:C:O2'    | 1:2:1684:U:O5'     | 2.13                     | 0.66              |
| 2:S0:185:ARG:HB2  | 23:D1:45:ALA:HB3   | 1.76                     | 0.66              |
| 4:S2:101:VAL:HG22 | 4:S2:115:ILE:HG12  | 1.76                     | 0.66              |
| 35:SM:34:LYS:NZ   | 36:1:2707:C:OP1    | 2.28                     | 0.66              |
| 47:M0:66:GLU:CD   | 47:M0:69:ARG:HH21  | 2.03                     | 0.66              |
| 1:6:482:U:H3      | 1:6:505:A:H61      | 1.42                     | 0.66              |
| 1:6:484:C:H42     | 1:6:503:G:H1       | 1.41                     | 0.66              |
| 24:d2:25:VAL:HG22 | 24:d2:65:LEU:HD21  | 1.78                     | 0.66              |
| 38:8:79:A:H3'     | 38:8:80:A:C8       | 2.30                     | 0.66              |
| 38:8:79:A:H2'     | 38:8:80:A:O4'      | 1.94                     | 0.66              |
| 41:l4:170:LYS:HG2 | 41:l4:175:HIS:HB2  | 1.77                     | 0.66              |
| 49:m3:89:TYR:CE1  | 49:m3:93:ILE:HD11  | 2.30                     | 0.66              |
| 1:2:1254:U:OP2    | 14:C2:46:ARG:NH1   | 2.27                     | 0.66              |
| 20:C8:145:ARG:HB2 | 35:SM:68:ARG:NH2   | 2.11                     | 0.66              |
| 56:N0:23:LYS:O    | 56:N0:24:LEU:HB2   | 1.95                     | 0.66              |
| 1:6:647:G:H22     | 1:6:687:G:N2       | 1.93                     | 0.66              |
| 39:l2:48:ILE:HD13 | 79:q3:65:ALA:HB2   | 1.78                     | 0.66              |
| 47:m0:14:ASN:O    | 47:m0:128:ARG:NH2  | 2.29                     | 0.66              |
| 51:m5:65:ARG:HG2  | 51:m5:127:TYR:CD1  | 2.29                     | 0.66              |
| 16:C4:81:VAL:H    | 16:C4:115:ILE:HG22 | 1.61                     | 0.66              |
| 36:1:2563:G:H5''  | 45:L8:27:THR:HG23  | 1.76                     | 0.66              |
| 36:1:3074:G:OP1   | 86:1:4042:OHX:N1   | 2.28                     | 0.66              |
| 40:l3:139:GLN:CB  | 40:l3:141:GLY:H    | 2.09                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:m0:24:ARG:HH11  | 47:m0:24:ARG:HG3   | 1.59                     | 0.66              |
| 1:2:301:A:OP2      | 86:2:2065:OHX:N2   | 2.28                     | 0.66              |
| 86:2:2032:OHX:N6   | 86:2:2147:OHX:N2   | 2.43                     | 0.66              |
| 4:S2:144:TRP:CE2   | 4:S2:173:PRO:HG3   | 2.31                     | 0.66              |
| 5:S3:32:GLU:OE1    | 5:S3:65:ARG:NH2    | 2.28                     | 0.66              |
| 29:D7:29:ARG:HG3   | 29:D7:29:ARG:NH1   | 2.10                     | 0.66              |
| 56:N0:2:ALA:HB3    | 56:N0:32:SER:HB3   | 1.78                     | 0.66              |
| 16:c4:107:ARG:HH21 | 16:c4:107:ARG:HB2  | 1.61                     | 0.66              |
| 36:5:715:A:H8      | 64:n8:115:LYS:HG3  | 1.60                     | 0.66              |
| 41:l4:140:HIS:NE2  | 41:l4:246:ARG:HG2  | 2.11                     | 0.66              |
| 59:n3:86:ARG:HG3   | 59:n3:92:PHE:CE2   | 2.30                     | 0.66              |
| 11:S9:129:ILE:HG12 | 11:S9:134:ILE:HD12 | 1.78                     | 0.66              |
| 18:C6:112:TYR:OH   | 18:C6:114:ARG:NH1  | 2.28                     | 0.66              |
| 28:D6:23:CYS:HB2   | 28:D6:74:CYS:HB3   | 1.78                     | 0.66              |
| 36:1:2227:C:OP1    | 78:Q2:32:LYS:NZ    | 2.28                     | 0.66              |
| 45:L8:54:GLU:HG2   | 45:L8:57:ARG:HH21  | 1.61                     | 0.66              |
| 56:N0:155:ARG:HD3  | 56:N0:172:TYR:CG   | 2.31                     | 0.66              |
| 2:s0:79:ARG:NH1    | 2:s0:164:ASN:O     | 2.27                     | 0.66              |
| 36:5:1249:G:H2'    | 36:5:1250:G:H8     | 1.61                     | 0.66              |
| 42:l5:148:ILE:HG23 | 42:l5:151:GLN:HB3  | 1.76                     | 0.66              |
| 1:2:1490:C:H4'     | 1:2:1491:U:OP1     | 1.94                     | 0.66              |
| 79:Q3:8:VAL:HB     | 79:Q3:11:THR:HG22  | 1.77                     | 0.66              |
| 40:l3:296:THR:CG2  | 40:l3:298:PHE:H    | 2.03                     | 0.66              |
| 60:n4:130:SER:HA   | 60:n4:133:THR:HG22 | 1.78                     | 0.66              |
| 1:2:1760:G:H2'     | 1:2:1761:U:H5'     | 1.78                     | 0.66              |
| 36:1:1235:U:H4'    | 36:1:1236:G:H5'    | 1.77                     | 0.66              |
| 36:1:3376:A:OP2    | 86:1:3911:OHX:N5   | 2.29                     | 0.66              |
| 46:L9:13:PRO:HD2   | 46:L9:16:VAL:HG22  | 1.78                     | 0.66              |
| 49:M3:64:LYS:HE3   | 64:N8:69:TRP:CD1   | 2.31                     | 0.66              |
| 34:sR:25:THR:OG1   | 34:sR:26:SER:N     | 2.28                     | 0.66              |
| 45:l8:144:GLU:OE1  | 72:o6:36:ARG:NH2   | 2.29                     | 0.66              |
| 36:1:2107:A:H2     | 36:1:3344:A:C8     | 2.14                     | 0.65              |
| 40:L3:102:LEU:HD23 | 40:L3:102:LEU:H    | 1.60                     | 0.65              |
| 74:O8:5:ILE:HG22   | 74:O8:54:LEU:HB2   | 1.78                     | 0.65              |
| 36:5:115:A:OP1     | 51:m5:49:ARG:NH2   | 2.29                     | 0.65              |
| 47:m0:86:HIS:HB3   | 47:m0:139:ARG:HG2  | 1.78                     | 0.65              |
| 1:2:565:C:O2       | 86:2:2040:OHX:N5   | 2.29                     | 0.65              |
| 36:1:1010:G:N2     | 47:M0:193:ASP:OD2  | 2.29                     | 0.65              |
| 36:1:3242:G:H21    | 36:1:3245:A:H5''   | 1.60                     | 0.65              |
| 86:1:3943:OHX:N5   | 86:1:4200:OHX:N2   | 2.43                     | 0.65              |
| 1:6:833:U:O4       | 86:6:2101:OHX:N2   | 2.30                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:s7:66:SER:O     | 9:s7:68:ALA:N      | 2.29                     | 0.65              |
| 44:l7:178:ILE:HA  | 44:l7:183:ASP:HB3  | 1.76                     | 0.65              |
| 1:2:66:U:C5       | 8:S6:173:PRO:HG3   | 2.30                     | 0.65              |
| 1:2:1796:C:C2     | 28:D6:5:ARG:HG2    | 2.31                     | 0.65              |
| 36:1:1213:G:OP1   | 56:N0:137:ARG:HD3  | 1.95                     | 0.65              |
| 36:1:1422:G:H21   | 43:L6:5:LYS:NZ     | 1.94                     | 0.65              |
| 36:1:2836:C:H5    | 36:1:2852:C:N4     | 1.94                     | 0.65              |
| 47:M0:74:LYS:O    | 47:M0:78:THR:HG23  | 1.96                     | 0.65              |
| 49:M3:174:ARG:HB2 | 72:O6:9:ILE:HD12   | 1.78                     | 0.65              |
| 36:5:3377:G:O6    | 86:5:4088:OHX:N2   | 2.28                     | 0.65              |
| 59:n3:2:SER:HA    | 59:n3:56:ASP:OD1   | 1.96                     | 0.65              |
| 1:2:1795:U:O2     | 28:D6:10:ARG:HD2   | 1.97                     | 0.65              |
| 36:1:1103:A:H1'   | 36:1:1104:G:OP1    | 1.96                     | 0.65              |
| 5:s3:179:GLN:OE1  | 5:s3:180:GLY:N     | 2.29                     | 0.65              |
| 19:c7:50:ILE:O    | 19:c7:54:THR:HG23  | 1.96                     | 0.65              |
| 36:5:299:G:N7     | 86:5:4187:OHX:N1   | 2.45                     | 0.65              |
| 36:5:2444:C:H42   | 36:5:2503:G:H1     | 1.43                     | 0.65              |
| 36:5:2996:U:H4'   | 36:5:2996:U:OP1    | 1.94                     | 0.65              |
| 30:D8:26:THR:HB   | 30:D8:44:VAL:HG22  | 1.77                     | 0.65              |
| 36:1:73:C:O2      | 49:M3:59:ARG:HD3   | 1.97                     | 0.65              |
| 36:1:2680:A:C2    | 48:M1:24:GLY:HA3   | 2.31                     | 0.65              |
| 36:5:497:C:O3'    | 69:o3:86:ARG:NH2   | 2.28                     | 0.65              |
| 36:5:912:G:OP2    | 39:l2:9:ARG:NH1    | 2.30                     | 0.65              |
| 36:5:2718:U:O4    | 86:5:4230:OHX:N6   | 2.29                     | 0.65              |
| 43:l6:31:ARG:NH1  | 69:o3:107:ILE:HG22 | 2.10                     | 0.65              |
| 1:2:420:A:OP1     | 8:S6:96:SER:OG     | 2.11                     | 0.65              |
| 1:2:1471:A:OP1    | 7:S5:185:ARG:NH1   | 2.30                     | 0.65              |
| 8:S6:57:ASP:HA    | 8:S6:106:LEU:HA    | 1.78                     | 0.65              |
| 47:M0:84:ALA:O    | 47:M0:140:THR:HG22 | 1.95                     | 0.65              |
| 1:6:1235:C:H5'    | 33:e1:146:SER:HB3  | 1.77                     | 0.65              |
| 2:s0:142:PRO:HB3  | 23:d1:34:ILE:HD13  | 1.78                     | 0.65              |
| 36:5:1764:U:H3'   | 36:5:1765:U:H5''   | 1.78                     | 0.65              |
| 36:5:2211:U:H5    | 36:5:2234:G:O6     | 1.79                     | 0.65              |
| 36:5:2407:C:H2'   | 36:5:2408:U:H6     | 1.62                     | 0.65              |
| 58:n2:19:VAL:HG12 | 58:n2:105:LEU:HD22 | 1.79                     | 0.65              |
| 1:2:734:A:H5''    | 1:2:735:C:OP1      | 1.96                     | 0.65              |
| 1:2:818:C:N4      | 1:2:819:G:O6       | 2.29                     | 0.65              |
| 9:S7:86:GLN:HG3   | 9:S7:87:ASP:H      | 1.62                     | 0.65              |
| 13:C1:5:LEU:O     | 13:C1:7:VAL:N      | 2.26                     | 0.65              |
| 36:1:3010:U:OP2   | 86:1:4203:OHX:N5   | 2.30                     | 0.65              |
| 39:L2:45:VAL:HG22 | 39:L2:84:THR:HA    | 1.79                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:L5:166:ALA:HB1  | 42:L5:171:LEU:HD12 | 1.79                     | 0.65              |
| 66:O0:13:LYS:HB3   | 66:O0:100:ILE:HG23 | 1.76                     | 0.65              |
| 86:5:4020:OHX:N6   | 86:5:4215:OHX:N2   | 2.44                     | 0.65              |
| 45:l8:33:ASN:O     | 45:l8:33:ASN:ND2   | 2.26                     | 0.65              |
| 72:o6:58:ILE:HG22  | 72:o6:90:MET:HG3   | 1.79                     | 0.65              |
| 1:2:57:G:OP1       | 26:D4:112:LYS:NZ   | 2.30                     | 0.65              |
| 3:S1:58:SER:HA     | 3:S1:62:LYS:HD3    | 1.78                     | 0.65              |
| 36:1:2310:U:OP1    | 86:1:4142:OHX:N2   | 2.29                     | 0.65              |
| 36:1:3276:G:N7     | 53:M7:171:ARG:NH1  | 2.44                     | 0.65              |
| 50:M4:37:GLU:HG3   | 50:M4:38:ILE:H     | 1.60                     | 0.65              |
| 10:s8:76:THR:HG21  | 10:s8:105:ASP:O    | 1.96                     | 0.65              |
| 15:c3:91:LEU:HD12  | 15:c3:125:LEU:HD12 | 1.78                     | 0.65              |
| 36:5:1329:U:H4'    | 36:5:1330:A:OP1    | 1.96                     | 0.65              |
| 66:o0:22:LYS:HD3   | 66:o0:94:GLU:HG3   | 1.77                     | 0.65              |
| 1:2:1760:G:C2'     | 1:2:1761:U:H5'     | 2.27                     | 0.65              |
| 40:L3:25:ILE:HD13  | 40:L3:25:ILE:H     | 1.62                     | 0.65              |
| 49:M3:64:LYS:HG3   | 64:N8:69:TRP:CG    | 2.32                     | 0.65              |
| 10:s8:76:THR:HG23  | 10:s8:108:PRO:HG2  | 1.78                     | 0.65              |
| 36:5:3274:A:H3'    | 36:5:3275:U:C5'    | 2.24                     | 0.65              |
| 1:2:568:G:N7       | 25:D3:69:ARG:NH2   | 2.45                     | 0.65              |
| 3:S1:129:THR:HA    | 3:S1:177:GLN:HA    | 1.78                     | 0.65              |
| 4:S2:234:PRO:O     | 4:S2:235:LEU:HB2   | 1.97                     | 0.65              |
| 12:C0:12:HIS:NE2   | 12:C0:49:LEU:HD21  | 2.11                     | 0.65              |
| 31:D9:33:LYS:O     | 31:D9:36:LEU:HD23  | 1.97                     | 0.65              |
| 86:6:2136:OHX:N3   | 10:s8:52:ASN:OD1   | 2.30                     | 0.65              |
| 36:5:1236:G:N2     | 36:5:1244:A:OP1    | 2.28                     | 0.65              |
| 36:5:2398:A:OP1    | 36:5:2873:U:H4'    | 1.96                     | 0.65              |
| 86:5:3973:OHX:N3   | 86:5:4241:OHX:N5   | 2.45                     | 0.65              |
| 34:SR:154:VAL:HG12 | 34:SR:171:SER:HB3  | 1.78                     | 0.64              |
| 36:1:709:A:OP1     | 54:M8:179:ARG:NH2  | 2.24                     | 0.64              |
| 43:L6:31:ARG:NH2   | 43:L6:81:ALA:O     | 2.29                     | 0.64              |
| 16:c4:11:SER:OG    | 16:c4:12:GLN:N     | 2.30                     | 0.64              |
| 36:5:540:U:H3      | 36:5:551:A:H61     | 1.45                     | 0.64              |
| 52:m6:65:ASN:OD1   | 52:m6:67:THR:HB    | 1.96                     | 0.64              |
| 1:2:325:G:H4'      | 13:C1:80:MET:HE3   | 1.79                     | 0.64              |
| 1:2:1502:G:O6      | 21:C9:102:ARG:NH2  | 2.30                     | 0.64              |
| 5:S3:178:ARG:HE    | 5:S3:178:ARG:H     | 1.45                     | 0.64              |
| 15:C3:26:PHE:HE2   | 15:C3:66:ILE:HD13  | 1.61                     | 0.64              |
| 36:1:118:U:O2      | 36:1:121:A:H5'     | 1.96                     | 0.64              |
| 36:1:1352:A:H4'    | 36:1:1353:U:OP1    | 1.98                     | 0.64              |
| 1:6:1239:U:O4      | 86:6:2097:OHX:N1   | 2.31                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:6:2121:OHX:N2   | 86:6:2171:OHX:N1   | 2.45                     | 0.64              |
| 2:s0:140:ASN:ND2   | 4:s2:62:PRO:HD3    | 2.12                     | 0.64              |
| 4:s2:45:VAL:HG21   | 4:s2:68:ILE:HG23   | 1.78                     | 0.64              |
| 7:s5:62:VAL:HG13   | 7:s5:89:ILE:HG12   | 1.79                     | 0.64              |
| 36:5:690:A:H4'     | 36:5:691:A:OP1     | 1.97                     | 0.64              |
| 42:l5:106:ALA:O    | 42:l5:110:LEU:HD22 | 1.97                     | 0.64              |
| 52:m6:12:LYS:O     | 56:n0:167:ARG:NH2  | 2.30                     | 0.64              |
| 1:2:142:G:N2       | 1:2:173:A:H2       | 1.95                     | 0.64              |
| 3:S1:110:LEU:HD11  | 3:S1:213:ARG:HD2   | 1.79                     | 0.64              |
| 5:S3:163:PRO:HA    | 5:S3:166:ASP:HB2   | 1.78                     | 0.64              |
| 36:1:1596:C:H2'    | 36:1:1597:C:C6     | 2.31                     | 0.64              |
| 63:N7:88:ASP:HB3   | 63:N7:121:ARG:HH22 | 1.62                     | 0.64              |
| 86:6:2121:OHX:N4   | 86:6:2171:OHX:N3   | 2.45                     | 0.64              |
| 43:l6:31:ARG:NH2   | 43:l6:81:ALA:O     | 2.31                     | 0.64              |
| 51:m5:119:TYR:OH   | 51:m5:131:GLU:OE1  | 2.13                     | 0.64              |
| 69:o3:59:VAL:HG23  | 69:o3:60:ARG:H     | 1.61                     | 0.64              |
| 1:2:159:U:O2'      | 8:S6:87:ARG:NH1    | 2.31                     | 0.64              |
| 36:1:563:U:OP1     | 56:N0:71:LYS:NZ    | 2.25                     | 0.64              |
| 36:1:718:G:C2      | 36:1:721:G:H1'     | 2.33                     | 0.64              |
| 36:1:2242:A:H5'    | 39:L2:243:THR:HG23 | 1.79                     | 0.64              |
| 40:L3:284:ARG:NH2  | 40:L3:295:ALA:O    | 2.23                     | 0.64              |
| 18:c6:95:LYS:O     | 34:sR:59:ARG:NH2   | 2.29                     | 0.64              |
| 47:m0:156:ARG:HG2  | 47:m0:163:GLN:HG2  | 1.79                     | 0.64              |
| 59:n3:2:SER:O      | 59:n3:57:MET:N     | 2.29                     | 0.64              |
| 59:n3:11:PHE:CG    | 59:n3:88:ARG:HD2   | 2.33                     | 0.64              |
| 1:2:73:U:H1'       | 1:2:74:U:H5'       | 1.80                     | 0.64              |
| 1:2:1367:G:N7      | 86:2:2109:OHX:N6   | 2.46                     | 0.64              |
| 30:D8:36:THR:OG1   | 30:D8:37:SER:N     | 2.25                     | 0.64              |
| 36:1:2767:U:OP2    | 86:1:4136:OHX:N2   | 2.31                     | 0.64              |
| 36:1:2897:A:H2'    | 36:1:2899:C:H5'    | 1.80                     | 0.64              |
| 37:3:49:G:C5       | 42:L5:58:LYS:HG3   | 2.32                     | 0.64              |
| 40:L3:41:VAL:HA    | 40:L3:185:GLY:HA3  | 1.79                     | 0.64              |
| 53:M7:59:PRO:HG3   | 53:M7:76:PHE:CD1   | 2.33                     | 0.64              |
| 34:sR:144:LEU:HD21 | 34:sR:186:PHE:HB3  | 1.78                     | 0.64              |
| 36:5:30:G:P        | 51:m5:172:ARG:HH11 | 2.21                     | 0.64              |
| 36:5:132:C:H2'     | 36:5:133:U:H5''    | 1.79                     | 0.64              |
| 36:5:1643:A:H4'    | 36:5:1822:C:H5'    | 1.79                     | 0.64              |
| 53:m7:53:ASP:O     | 86:m7:206:OHX:N6   | 2.30                     | 0.64              |
| 1:2:190:C:N4       | 1:2:196:G:O6       | 2.31                     | 0.64              |
| 18:C6:38:LEU:O     | 18:C6:40:GLU:N     | 2.30                     | 0.64              |
| 1:6:151:G:N2       | 1:6:163:G:N2       | 2.45                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:6:1034:C:HO2'   | 24:d2:2:THR:N      | 1.96                     | 0.64              |
| 1:6:1058:U:H4'    | 1:6:1059:U:OP1     | 1.97                     | 0.64              |
| 36:5:498:A:H5'    | 69:o3:86:ARG:NH1   | 2.12                     | 0.64              |
| 36:5:980:A:H2'    | 36:5:981:U:C2      | 2.33                     | 0.64              |
| 39:l2:45:VAL:HG22 | 39:l2:84:THR:HA    | 1.80                     | 0.64              |
| 47:m0:99:ILE:HG13 | 47:m0:123:HIS:HB2  | 1.79                     | 0.64              |
| 1:2:702:G:O2'     | 1:2:703:G:H8       | 1.80                     | 0.64              |
| 1:2:740:A:C2'     | 1:2:741:C:H5''     | 2.28                     | 0.64              |
| 33:E1:135:HIS:HB2 | 33:E1:138:ARG:HB3  | 1.80                     | 0.64              |
| 36:1:1613:A:OP2   | 74:O8:46:ARG:NH2   | 2.30                     | 0.64              |
| 54:M8:158:HIS:H   | 54:M8:186:VAL:CG1  | 2.11                     | 0.64              |
| 1:6:159:U:O2'     | 8:s6:87:ARG:NH1    | 2.31                     | 0.64              |
| 19:c7:104:ASN:O   | 19:c7:106:THR:N    | 2.30                     | 0.64              |
| 36:5:528:U:H2'    | 36:5:529:A:C8      | 2.32                     | 0.64              |
| 36:5:1952:G:H1    | 36:5:2094:C:H42    | 1.46                     | 0.64              |
| 46:l9:86:TYR:CE2  | 46:l9:151:VAL:HG22 | 2.32                     | 0.64              |
| 52:m6:182:ASN:OD1 | 52:m6:186:ALA:HB2  | 1.98                     | 0.64              |
| 5:S3:94:ARG:NH2   | 35:SM:134:ASP:OD1  | 2.23                     | 0.64              |
| 36:1:12:A:OP1     | 86:1:4205:OHX:N6   | 2.31                     | 0.64              |
| 36:1:595:G:H1     | 36:1:609:G:H5''    | 1.63                     | 0.64              |
| 44:L7:26:VAL:HG23 | 44:L7:27:ALA:H     | 1.63                     | 0.64              |
| 86:6:2121:OHX:N2  | 86:6:2171:OHX:N5   | 2.45                     | 0.64              |
| 86:7:218:OHX:N3   | 86:7:226:OHX:N5    | 2.45                     | 0.64              |
| 26:D4:3:ASP:O     | 26:D4:5:VAL:N      | 2.30                     | 0.64              |
| 36:1:2573:G:O6    | 86:1:4002:OHX:N3   | 2.30                     | 0.64              |
| 59:N3:13:ILE:HG22 | 59:N3:85:TRP:CD1   | 2.33                     | 0.64              |
| 66:O0:15:ALA:O    | 66:O0:18:ILE:HG22  | 1.98                     | 0.64              |
| 34:sR:38:ARG:HG2  | 34:sR:67:ILE:HG23  | 1.80                     | 0.64              |
| 36:5:18:G:OP1     | 71:o5:81:ARG:NH2   | 2.29                     | 0.64              |
| 39:l2:172:GLY:HA3 | 79:q3:68:ALA:H     | 1.63                     | 0.64              |
| 52:m6:62:THR:H    | 52:m6:69:GLY:HA3   | 1.62                     | 0.64              |
| 1:2:260:U:H3'     | 1:2:261:U:H5''     | 1.78                     | 0.64              |
| 2:S0:63:ILE:HG12  | 23:D1:36:VAL:HG22  | 1.80                     | 0.64              |
| 21:C9:42:GLY:HA2  | 21:C9:84:LYS:HB2   | 1.80                     | 0.64              |
| 36:1:13:A:OP2     | 86:1:4205:OHX:N5   | 2.30                     | 0.64              |
| 36:1:917:A:OP2    | 86:1:4146:OHX:N2   | 2.31                     | 0.64              |
| 36:1:1507:G:N7    | 53:M7:129:THR:HG22 | 2.12                     | 0.64              |
| 36:1:2278:C:OP1   | 77:Q1:23:ARG:NH1   | 2.31                     | 0.64              |
| 45:L8:156:ASP:OD2 | 45:L8:156:ASP:N    | 2.30                     | 0.64              |
| 9:s7:130:VAL:HG11 | 9:s7:154:LEU:HD21  | 1.80                     | 0.64              |
| 36:5:284:A:OP2    | 78:q2:41:ARG:NH1   | 2.28                     | 0.64              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:3128:G:OP2    | 86:5:4157:OHX:N3   | 2.31                     | 0.64              |
| 62:n6:91:ASN:O     | 62:n6:93:ALA:N     | 2.31                     | 0.64              |
| 1:2:1034:C:HO2'    | 24:D2:2:THR:N      | 1.96                     | 0.63              |
| 3:S1:51:SER:HA     | 3:S1:57:ALA:H      | 1.61                     | 0.63              |
| 9:S7:131:PHE:O     | 9:S7:133:THR:N     | 2.31                     | 0.63              |
| 28:D6:84:VAL:O     | 28:D6:86:VAL:N     | 2.31                     | 0.63              |
| 34:SR:33:LEU:HB3   | 34:SR:45:TRP:HB2   | 1.79                     | 0.63              |
| 36:1:2209:U:O2'    | 36:1:2210:G:OP1    | 2.14                     | 0.63              |
| 36:1:2554:A:N7     | 79:Q3:62:LYS:NZ    | 2.45                     | 0.63              |
| 1:6:656:G:N2       | 1:6:675:U:O2       | 2.31                     | 0.63              |
| 1:6:1793:G:O2'     | 28:d6:5:ARG:NH2    | 2.31                     | 0.63              |
| 30:d8:10:ALA:HB1   | 30:d8:30:VAL:HB    | 1.78                     | 0.63              |
| 86:7:218:OHX:N1    | 86:7:226:OHX:N5    | 2.47                     | 0.63              |
| 39:l2:204:MET:HE3  | 39:l2:208:ASP:HB2  | 1.80                     | 0.63              |
| 7:S5:43:PHE:CZ     | 7:S5:90:ILE:HG21   | 2.33                     | 0.63              |
| 18:C6:126:PRO:O    | 18:C6:128:LYS:NZ   | 2.26                     | 0.63              |
| 1:6:1564:U:H2'     | 1:6:1565:C:C6      | 2.34                     | 0.63              |
| 21:c9:139:THR:O    | 21:c9:142:GLU:HG3  | 1.98                     | 0.63              |
| 44:l7:96:PRO:O     | 44:l7:99:PRO:HD2   | 1.98                     | 0.63              |
| 2:S0:70:PRO:HB2    | 2:S0:94:GLY:HA3    | 1.79                     | 0.63              |
| 11:S9:163:PRO:O    | 11:S9:165:GLY:N    | 2.31                     | 0.63              |
| 44:L7:244:ASN:HD22 | 44:L7:244:ASN:C    | 2.06                     | 0.63              |
| 63:N7:95:VAL:HG21  | 63:N7:113:VAL:HG11 | 1.78                     | 0.63              |
| 1:6:339:C:OP2      | 10:s8:10:LYS:NZ    | 2.29                     | 0.63              |
| 2:s0:56:LYS:HE3    | 2:s0:158:VAL:HG23  | 1.79                     | 0.63              |
| 7:s5:225:ARG:NH2   | 30:d8:58:GLU:HB2   | 2.13                     | 0.63              |
| 9:s7:117:THR:HG22  | 9:s7:120:ALA:H     | 1.62                     | 0.63              |
| 36:5:990:U:O4      | 86:5:4182:OHX:N6   | 2.31                     | 0.63              |
| 36:5:1308:A:OP2    | 36:5:1308:A:C8     | 2.52                     | 0.63              |
| 36:5:1878:G:O2'    | 36:5:1879:A:OP1    | 2.16                     | 0.63              |
| 36:5:1881:A:OP2    | 86:5:4030:OHX:N6   | 2.31                     | 0.63              |
| 72:o6:57:LEU:O     | 72:o6:61:ILE:HG12  | 1.97                     | 0.63              |
| 82:p0:91:GLU:HG2   | 82:p0:92:PRO:HD2   | 1.78                     | 0.63              |
| 1:2:45:U:O2'       | 1:2:46:A:H2'       | 1.99                     | 0.63              |
| 3:S1:111:ARG:HB3   | 28:D6:68:TYR:CD2   | 2.33                     | 0.63              |
| 18:C6:32:ASN:N     | 18:C6:67:VAL:O     | 2.25                     | 0.63              |
| 36:1:410:U:O4      | 86:1:4060:OHX:N5   | 2.30                     | 0.63              |
| 46:L9:84:LYS:HE2   | 46:L9:191:LEU:HD13 | 1.79                     | 0.63              |
| 67:O1:19:ARG:HD3   | 67:O1:35:GLU:HG3   | 1.80                     | 0.63              |
| 8:s6:199:GLN:O     | 8:s6:203:GLU:HG3   | 1.98                     | 0.63              |
| 15:c3:26:PHE:CE2   | 15:c3:28:LEU:HB2   | 2.34                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:sR:19:TRP:HB2  | 34:sR:38:ARG:HG3   | 1.80                     | 0.63              |
| 36:5:1345:G:N7    | 86:5:4066:OHX:N5   | 2.45                     | 0.63              |
| 86:5:4020:OHX:N3  | 86:5:4215:OHX:N1   | 2.47                     | 0.63              |
| 54:m8:170:ARG:O   | 54:m8:171:LYS:HB2  | 1.97                     | 0.63              |
| 2:S0:150:ASP:OD1  | 2:S0:165:ARG:NH2   | 2.25                     | 0.63              |
| 22:D0:20:ILE:HD13 | 22:D0:22:ILE:HD13  | 1.80                     | 0.63              |
| 36:1:272:G:OP2    | 86:1:4034:OHX:N3   | 2.31                     | 0.63              |
| 36:1:979:U:C2     | 36:1:980:A:C4      | 2.87                     | 0.63              |
| 42:L5:187:THR:O   | 42:L5:189:GLU:N    | 2.31                     | 0.63              |
| 46:L9:48:VAL:HG13 | 46:L9:52:LEU:HB3   | 1.81                     | 0.63              |
| 1:6:151:G:H22     | 1:6:163:G:N2       | 1.96                     | 0.63              |
| 1:6:546:U:H2'     | 1:6:547:U:C6       | 2.34                     | 0.63              |
| 1:6:987:G:O6      | 86:6:2120:OHX:N4   | 2.32                     | 0.63              |
| 1:6:1160:A:H2'    | 1:6:1161:C:C6      | 2.33                     | 0.63              |
| 7:s5:140:THR:HA   | 7:s5:214:LYS:HD2   | 1.80                     | 0.63              |
| 36:5:304:G:N3     | 36:5:304:G:H5'     | 2.12                     | 0.63              |
| 38:8:136:G:OP1    | 61:n5:48:SER:OG    | 2.13                     | 0.63              |
| 3:S1:109:LYS:HG3  | 3:S1:113:MET:HE3   | 1.79                     | 0.63              |
| 9:S7:44:LYS:NZ    | 9:S7:95:GLU:HG2    | 2.13                     | 0.63              |
| 33:E1:144:CYS:HB3 | 33:E1:147:VAL:HG13 | 1.81                     | 0.63              |
| 34:SR:136:ILE:H   | 34:SR:136:ILE:HD13 | 1.64                     | 0.63              |
| 36:1:3169:U:H2'   | 36:1:3170:A:O4'    | 1.99                     | 0.63              |
| 36:5:2202:C:O4'   | 39:l2:224:THR:HG23 | 1.98                     | 0.63              |
| 36:5:3047:U:O2'   | 36:5:3048:A:H5'    | 1.98                     | 0.63              |
| 57:n1:32:LYS:HE3  | 57:n1:98:HIS:HD2   | 1.62                     | 0.63              |
| 82:p0:4:ILE:HD13  | 82:p0:4:ILE:H      | 1.63                     | 0.63              |
| 1:2:1600:A:H4'    | 1:2:1601:G:OP1     | 1.98                     | 0.63              |
| 3:S1:157:GLN:H    | 3:S1:160:HIS:HB2   | 1.64                     | 0.63              |
| 36:1:883:A:H5'    | 53:M7:133:HIS:HA   | 1.80                     | 0.63              |
| 36:1:2403:G:N2    | 36:1:2404:A:H62    | 1.97                     | 0.63              |
| 38:4:135:G:OP2    | 61:N5:56:ARG:NH2   | 2.31                     | 0.63              |
| 1:6:194:U:O2      | 1:6:195:G:O2'      | 2.15                     | 0.63              |
| 1:6:1579:U:OP1    | 86:6:2182:OHX:N4   | 2.32                     | 0.63              |
| 1:2:1114:G:O6     | 86:2:2075:OHX:N5   | 2.32                     | 0.63              |
| 8:S6:98:ARG:NH2   | 8:S6:101:ILE:O     | 2.32                     | 0.63              |
| 16:C4:85:ALA:H    | 16:C4:119:THR:CG2  | 2.12                     | 0.63              |
| 2:s0:11:PRO:O     | 2:s0:15:GLN:HG3    | 1.99                     | 0.63              |
| 20:c8:145:ARG:HD3 | 35:sM:68:ARG:NE    | 2.14                     | 0.63              |
| 36:5:739:G:O6     | 86:5:3966:OHX:N6   | 2.31                     | 0.63              |
| 36:5:1655:G:H5'   | 36:5:1655:G:H8     | 1.62                     | 0.63              |
| 36:5:2341:A:OP2   | 40:l3:247:ARG:NH2  | 2.32                     | 0.63              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:m4:19:ARG:HA    | 50:m4:69:THR:HG22  | 1.81                     | 0.63              |
| 61:n5:115:ARG:HH11 | 61:n5:115:ARG:HG3  | 1.64                     | 0.63              |
| 1:2:794:U:O2'      | 1:2:795:U:O2       | 2.10                     | 0.63              |
| 36:1:1176:C:OP1    | 52:M6:25:LYS:HE3   | 1.99                     | 0.63              |
| 36:1:1243:G:N2     | 36:1:1244:A:N7     | 2.47                     | 0.63              |
| 36:1:1724:U:H4'    | 36:1:1725:C:OP1    | 1.99                     | 0.63              |
| 36:1:3259:U:H6     | 36:1:3259:U:H5'    | 1.64                     | 0.63              |
| 40:L3:92:TYR:O     | 40:L3:155:ALA:HA   | 1.98                     | 0.63              |
| 57:N1:17:ARG:O     | 57:N1:18:ASP:HB2   | 1.98                     | 0.63              |
| 2:s0:163:ASN:O     | 2:s0:165:ARG:N     | 2.32                     | 0.63              |
| 36:1:1286:A:N3     | 36:1:1287:A:H1'    | 2.14                     | 0.62              |
| 42:L5:155:THR:HG22 | 42:L5:179:ARG:NH1  | 2.14                     | 0.62              |
| 63:N7:83:THR:HG23  | 63:N7:85:TYR:H     | 1.63                     | 0.62              |
| 7:s5:90:ILE:O      | 7:s5:94:THR:HG23   | 1.98                     | 0.62              |
| 31:d9:21:CYS:HB2   | 31:d9:39:CYS:HB3   | 1.81                     | 0.62              |
| 36:5:1817:G:OP1    | 86:5:4178:OHX:N1   | 2.31                     | 0.62              |
| 36:5:2676:A:H4'    | 36:5:2677:G:O5'    | 1.99                     | 0.62              |
| 38:8:143:U:OP1     | 51:m5:38:ARG:NH2   | 2.31                     | 0.62              |
| 40:l3:41:VAL:CA    | 40:l3:185:GLY:HA3  | 2.26                     | 0.62              |
| 42:l5:64:ILE:HG13  | 42:l5:109:THR:HG21 | 1.80                     | 0.62              |
| 68:o2:123:LYS:HA   | 68:o2:126:LEU:HD12 | 1.80                     | 0.62              |
| 86:2:2091:OHX:N3   | 86:2:2132:OHX:N6   | 2.47                     | 0.62              |
| 19:C7:17:ILE:HG23  | 19:C7:58:MET:HE2   | 1.80                     | 0.62              |
| 25:D3:126:LYS:HA   | 25:D3:131:SER:HA   | 1.81                     | 0.62              |
| 36:1:276:U:O2      | 51:M5:93:LYS:NZ    | 2.32                     | 0.62              |
| 36:1:1014:U:H2'    | 36:1:1015:U:H5''   | 1.79                     | 0.62              |
| 36:1:1308:A:C8     | 36:1:1308:A:OP2    | 2.52                     | 0.62              |
| 48:M1:108:GLU:HG2  | 48:M1:122:ILE:HG21 | 1.81                     | 0.62              |
| 1:6:486:G:O6       | 1:6:488:G:N2       | 2.32                     | 0.62              |
| 1:6:1690:G:H1      | 1:6:1711:C:H42     | 1.47                     | 0.62              |
| 11:s9:157:ASP:OD1  | 11:s9:158:PHE:N    | 2.31                     | 0.62              |
| 13:c1:33:ARG:HH22  | 13:c1:51:GLY:C     | 2.07                     | 0.62              |
| 36:5:59:G:H2'      | 38:8:33:A:O2'      | 1.99                     | 0.62              |
| 46:l9:129:ARG:O    | 46:l9:132:VAL:HG13 | 1.99                     | 0.62              |
| 70:o4:16:ARG:HH11  | 70:o4:16:ARG:HG3   | 1.63                     | 0.62              |
| 86:2:2040:OHX:N1   | 25:D3:64:PRO:O     | 2.32                     | 0.62              |
| 2:S0:124:THR:HG22  | 2:S0:174:TRP:HE1   | 1.64                     | 0.62              |
| 66:O0:24:THR:HG22  | 66:O0:91:SER:HB3   | 1.80                     | 0.62              |
| 67:O1:36:ILE:HD12  | 67:O1:59:ILE:HD11  | 1.81                     | 0.62              |
| 1:6:375:U:OP1      | 25:d3:23:ARG:NH2   | 2.30                     | 0.62              |
| 1:6:1783:C:OP2     | 77:q1:1:MET:HB2    | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:c8:35:ILE:HB   | 20:c8:38:VAL:HG22 | 1.81                     | 0.62              |
| 22:d0:18:GLN:O    | 22:d0:96:PRO:HB3  | 2.00                     | 0.62              |
| 50:m4:48:GLY:HA3  | 50:m4:53:VAL:HG13 | 1.81                     | 0.62              |
| 1:2:434:G:N7      | 86:2:2049:OHX:N4  | 2.46                     | 0.62              |
| 1:2:649:U:O2'     | 1:2:650:U:O5'     | 2.17                     | 0.62              |
| 6:S4:31:PRO:HG2   | 6:S4:38:LEU:HD13  | 1.80                     | 0.62              |
| 36:1:1846:C:OP1   | 36:1:1849:C:N4    | 2.31                     | 0.62              |
| 47:M0:73:ASN:O    | 47:M0:77:THR:HG23 | 1.98                     | 0.62              |
| 48:M1:59:ILE:HG21 | 48:M1:65:ILE:HD11 | 1.80                     | 0.62              |
| 1:6:86:A:OP2      | 86:6:2188:OHX:N1  | 2.33                     | 0.62              |
| 10:s8:76:THR:HG22 | 10:s8:105:ASP:HB3 | 1.81                     | 0.62              |
| 36:5:438:A:C8     | 36:5:439:C:H5     | 2.17                     | 0.62              |
| 86:5:4020:OHX:N5  | 86:5:4215:OHX:N2  | 2.47                     | 0.62              |
| 47:m0:86:HIS:HB3  | 47:m0:139:ARG:CG  | 2.30                     | 0.62              |
| 1:2:1595:U:N3     | 1:2:1600:A:H2     | 1.97                     | 0.62              |
| 5:S3:170:THR:HG22 | 5:S3:187:LYS:HG2  | 1.80                     | 0.62              |
| 12:C0:15:LEU:HD22 | 12:C0:46:LEU:HD11 | 1.81                     | 0.62              |
| 34:SR:64:HIS:ND1  | 34:SR:86:ASP:OD2  | 2.31                     | 0.62              |
| 36:1:2663:G:H5'   | 42:L5:152:ARG:HD3 | 1.81                     | 0.62              |
| 44:L7:176:TYR:CZ  | 44:L7:197:GLN:HG2 | 2.34                     | 0.62              |
| 53:M7:84:PRO:HB2  | 53:M7:87:SER:HB2  | 1.81                     | 0.62              |
| 12:c0:58:GLN:HB3  | 12:c0:65:TYR:HB2  | 1.80                     | 0.62              |
| 36:5:838:G:O6     | 79:q3:4:ARG:NH2   | 2.32                     | 0.62              |
| 36:5:1093:A:OP1   | 36:5:1093:A:H4'   | 1.98                     | 0.62              |
| 36:5:2818:U:H5'   | 36:5:2818:U:C6    | 2.33                     | 0.62              |
| 42:l5:261:THR:H   | 42:l5:264:GLN:NE2 | 1.96                     | 0.62              |
| 1:2:533:U:H4'     | 26:D4:33:ALA:HB2  | 1.81                     | 0.62              |
| 4:S2:103:VAL:HG12 | 4:S2:190:LEU:HD12 | 1.81                     | 0.62              |
| 5:S3:40:ARG:HG2   | 22:D0:110:PRO:HB3 | 1.81                     | 0.62              |
| 5:S3:195:SER:O    | 5:S3:197:THR:N    | 2.29                     | 0.62              |
| 10:S8:8:ARG:HD3   | 10:S8:21:PHE:HB3  | 1.80                     | 0.62              |
| 36:1:2534:G:H2'   | 36:1:2535:A:H8    | 1.65                     | 0.62              |
| 41:L4:9:HIS:CE1   | 41:L4:146:PRO:HB2 | 2.35                     | 0.62              |
| 52:M6:65:ASN:OD1  | 52:M6:67:THR:HB   | 1.99                     | 0.62              |
| 1:6:837:G:O6      | 86:6:2101:OHX:N1  | 2.31                     | 0.62              |
| 3:s1:126:THR:HG22 | 3:s1:136:ARG:HE   | 1.65                     | 0.62              |
| 17:c5:12:PHE:CZ   | 48:m1:85:LYS:HE2  | 2.34                     | 0.62              |
| 36:5:2128:C:OP1   | 86:5:4090:OHX:N3  | 2.33                     | 0.62              |
| 36:5:3170:A:OP2   | 69:o3:56:SER:OG   | 2.11                     | 0.62              |
| 37:7:2:G:O2'      | 37:7:23:A:N1      | 2.31                     | 0.62              |
| 45:l8:163:VAL:O   | 45:l8:166:LEU:HB2 | 2.00                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:m6:10:ASP:OD2  | 52:m6:37:ARG:NH2   | 2.27                     | 0.62              |
| 66:o0:26:GLY:O    | 66:o0:30:THR:HG23  | 2.00                     | 0.62              |
| 70:o4:42:PRO:HB2  | 70:o4:51:LEU:HD12  | 1.81                     | 0.62              |
| 1:2:25:C:OP2      | 1:2:25:C:H4'       | 2.00                     | 0.62              |
| 86:2:2162:OHX:N4  | 8:S6:155:ASP:OD1   | 2.33                     | 0.62              |
| 36:1:837:A:OP1    | 79:Q3:5:THR:OG1    | 2.14                     | 0.62              |
| 36:1:2717:U:OP1   | 86:1:3987:OHX:N6   | 2.33                     | 0.62              |
| 38:4:107:G:OP2    | 86:4:232:OHX:N2    | 2.33                     | 0.62              |
| 50:M4:60:LEU:HD13 | 56:N0:152:LEU:HD11 | 1.81                     | 0.62              |
| 2:s0:41:ARG:NH1   | 2:s0:45:VAL:HG21   | 2.12                     | 0.62              |
| 36:5:1481:A:O4'   | 36:5:1481:A:OP1    | 2.18                     | 0.62              |
| 39:l2:204:MET:CE  | 39:l2:209:HIS:HB2  | 2.26                     | 0.62              |
| 1:2:434:G:H5'     | 25:D3:78:LYS:HB3   | 1.82                     | 0.62              |
| 1:2:730:G:O6      | 86:2:2157:OHX:N4   | 2.33                     | 0.62              |
| 1:2:1382:A:H5''   | 22:D0:60:THR:HG22  | 1.82                     | 0.62              |
| 5:S3:105:MET:HG2  | 5:S3:122:VAL:HG21  | 1.80                     | 0.62              |
| 5:S3:178:ARG:H    | 5:S3:178:ARG:NE    | 1.98                     | 0.62              |
| 34:SR:295:SER:HB2 | 34:SR:300:THR:HB   | 1.81                     | 0.62              |
| 36:1:2108:C:H1'   | 36:1:3344:A:C8     | 2.35                     | 0.62              |
| 1:6:568:G:N7      | 25:d3:69:ARG:NH2   | 2.47                     | 0.62              |
| 33:e1:82:LYS:O    | 33:e1:84:VAL:N     | 2.31                     | 0.62              |
| 36:5:1765:U:H4'   | 36:5:1765:U:OP1    | 1.99                     | 0.62              |
| 36:5:3215:A:O5'   | 50:m4:121:MET:HE1  | 1.99                     | 0.62              |
| 41:l4:139:GLY:O   | 41:l4:180:LYS:HE2  | 1.99                     | 0.62              |
| 1:2:591:A:H2'     | 1:2:592:A:C8       | 2.35                     | 0.62              |
| 3:S1:212:VAL:O    | 3:S1:214:LYS:N     | 2.32                     | 0.62              |
| 10:S8:163:GLY:HA3 | 36:1:3354:U:H1'    | 1.82                     | 0.62              |
| 36:1:1541:G:OP2   | 86:1:4023:OHX:N5   | 2.33                     | 0.62              |
| 36:1:3393:U:H2'   | 36:1:3394:U:C6     | 2.34                     | 0.62              |
| 43:L6:158:TYR:OH  | 50:M4:114:ASP:OD2  | 2.17                     | 0.62              |
| 54:M8:34:THR:HG22 | 54:M8:49:LEU:HD21  | 1.82                     | 0.62              |
| 6:s4:62:LYS:NZ    | 6:s4:66:MET:HE3    | 2.15                     | 0.62              |
| 11:s9:29:LYS:O    | 11:s9:33:GLU:HG2   | 1.99                     | 0.62              |
| 17:c5:25:LEU:HA   | 17:c5:28:MET:HE2   | 1.81                     | 0.62              |
| 17:c5:119:PHE:HE1 | 20:c8:119:ILE:HG23 | 1.65                     | 0.62              |
| 27:d5:82:HIS:O    | 27:d5:85:LYS:N     | 2.32                     | 0.62              |
| 36:5:3212:C:OP2   | 50:m4:124:ARG:NH2  | 2.33                     | 0.62              |
| 86:7:218:OHX:N4   | 86:7:226:OHX:N2    | 2.47                     | 0.62              |
| 41:l4:20:LEU:HD11 | 41:l4:252:GLU:HG3  | 1.81                     | 0.62              |
| 52:m6:16:VAL:CG2  | 52:m6:43:ILE:HG12  | 2.30                     | 0.62              |
| 68:o2:16:LYS:O    | 68:o2:17:PHE:HB2   | 2.00                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:359:A:C2     | 25:D3:38:PHE:HB3  | 2.34                     | 0.62              |
| 5:S3:48:VAL:HB   | 5:S3:86:LEU:HD12  | 1.81                     | 0.62              |
| 13:C1:80:MET:HB3 | 13:C1:83:THR:HG23 | 1.81                     | 0.62              |
| 36:1:735:A:H2'   | 36:1:736:A:C8     | 2.34                     | 0.62              |
| 36:1:2572:C:O2'  | 36:1:2573:G:O4'   | 2.18                     | 0.62              |
| 36:1:2741:C:O2'  | 78:Q2:20:HIS:ND1  | 2.33                     | 0.62              |
| 48:M1:50:ALA:HB2 | 48:M1:65:ILE:HD12 | 1.82                     | 0.62              |
| 67:O1:79:ARG:HA  | 67:O1:89:LEU:HD12 | 1.81                     | 0.62              |
| 75:O9:44:TRP:CZ3 | 75:O9:45:ARG:HG3  | 2.35                     | 0.62              |
| 78:Q2:99:GLN:OE1 | 78:Q2:102:GLN:NE2 | 2.25                     | 0.62              |
| 1:6:105:A:OP1    | 10:s8:18:ARG:NH1  | 2.33                     | 0.62              |
| 1:6:823:G:H2'    | 1:6:824:G:O4'     | 1.98                     | 0.62              |
| 1:6:1239:U:O2    | 1:6:1246:C:N4     | 2.33                     | 0.62              |
| 1:6:1776:A:H2'   | 1:6:1777:G:C8     | 2.35                     | 0.62              |
| 3:s1:154:SER:O   | 3:s1:154:SER:OG   | 2.15                     | 0.62              |
| 4:s2:132:ALA:O   | 4:s2:135:SER:OG   | 2.12                     | 0.62              |
| 23:d1:9:VAL:HG22 | 23:d1:10:GLU:H    | 1.64                     | 0.62              |
| 25:d3:126:LYS:HA | 25:d3:131:SER:HA  | 1.81                     | 0.62              |
| 36:5:911:C:H42   | 39:l2:3:ARG:HD3   | 1.64                     | 0.62              |
| 36:5:924:G:OP1   | 86:5:4212:OHX:N4  | 2.33                     | 0.62              |
| 36:5:1025:A:H3'  | 36:5:1026:A:H4'   | 1.82                     | 0.62              |
| 2:S0:185:ARG:HG3 | 23:D1:47:PRO:HD3  | 1.81                     | 0.61              |
| 36:1:562:C:H2'   | 36:1:563:U:C6     | 2.35                     | 0.61              |
| 36:1:2867:C:H6   | 36:1:2867:C:H5'   | 1.65                     | 0.61              |
| 1:6:476:U:OP1    | 1:6:477:A:O2'     | 2.17                     | 0.61              |
| 1:6:833:U:O4     | 86:6:2101:OHX:N5  | 2.33                     | 0.61              |
| 16:c4:25:ASP:OD1 | 16:c4:26:THR:N    | 2.32                     | 0.61              |
| 34:sR:22:SER:OG  | 34:sR:70:ASP:HA   | 2.00                     | 0.61              |
| 36:5:1024:G:N7   | 36:5:1027:A:N6    | 2.47                     | 0.61              |
| 36:5:2761:G:N7   | 78:q2:63:LYS:NZ   | 2.47                     | 0.61              |
| 38:8:135:G:OP2   | 61:n5:56:ARG:NH2  | 2.33                     | 0.61              |
| 51:m5:46:ASP:OD1 | 51:m5:50:ARG:NH2  | 2.33                     | 0.61              |
| 1:2:1234:A:H4'   | 33:E1:146:SER:HB3 | 1.82                     | 0.61              |
| 13:C1:59:PRO:HG2 | 13:C1:60:PHE:CE2  | 2.35                     | 0.61              |
| 20:C8:94:ASP:OD1 | 20:C8:98:TYR:OH   | 2.15                     | 0.61              |
| 36:1:807:A:H61   | 36:1:934:G:H22    | 1.48                     | 0.61              |
| 36:1:3047:U:O2'  | 40:L3:53:MET:HE1  | 1.99                     | 0.61              |
| 73:O7:88:ALA:O   | 86:O7:103:OHX:N4  | 2.33                     | 0.61              |
| 1:6:770:A:OP2    | 86:6:2138:OHX:N3  | 2.33                     | 0.61              |
| 1:6:1568:C:OP1   | 20:c8:36:LYS:NZ   | 2.28                     | 0.61              |
| 52:m6:61:ALA:HB1 | 52:m6:66:LYS:HG3  | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:706:A:N1       | 1:2:734:A:N6       | 2.49                     | 0.61              |
| 1:2:1450:U:OP2     | 86:2:2063:OHX:N5   | 2.33                     | 0.61              |
| 1:2:1650:U:H2'     | 1:2:1651:A:C8      | 2.35                     | 0.61              |
| 36:1:1808:G:O6     | 86:1:3986:OHX:N3   | 2.34                     | 0.61              |
| 36:1:2697:A:H2'    | 36:1:2698:G:C8     | 2.36                     | 0.61              |
| 86:1:4007:OHX:N6   | 86:1:4175:OHX:N1   | 2.48                     | 0.61              |
| 45:L8:101:THR:HG23 | 45:L8:104:GLU:H    | 1.65                     | 0.61              |
| 46:L9:171:ASP:OD2  | 46:L9:173:ARG:NH1  | 2.33                     | 0.61              |
| 1:6:104:A:OP2      | 1:6:308:C:N4       | 2.31                     | 0.61              |
| 1:6:213:A:OP2      | 86:6:2150:OHX:N1   | 2.32                     | 0.61              |
| 2:s0:185:ARG:H     | 23:d1:45:ALA:H     | 1.46                     | 0.61              |
| 7:s5:133:VAL:HG22  | 7:s5:198:LEU:HD13  | 1.81                     | 0.61              |
| 33:e1:90:LYS:HB2   | 33:e1:93:HIS:CE1   | 2.35                     | 0.61              |
| 36:5:353:G:N7      | 73:o7:55:ARG:HD3   | 2.15                     | 0.61              |
| 36:5:1322:U:O2     | 56:n0:108:GLN:NE2  | 2.33                     | 0.61              |
| 86:7:218:OHX:N4    | 86:7:226:OHX:N6    | 2.49                     | 0.61              |
| 41:l4:98:ARG:HD2   | 41:l4:99:MET:O     | 1.99                     | 0.61              |
| 43:l6:40:LEU:HD11  | 43:l6:54:TYR:HB2   | 1.82                     | 0.61              |
| 49:m3:80:VAL:HG12  | 49:m3:85:LEU:O     | 2.00                     | 0.61              |
| 1:2:741:C:O2       | 9:S7:107:ARG:NH1   | 2.25                     | 0.61              |
| 1:2:780:A:C8       | 26:D4:8:ARG:HB3    | 2.35                     | 0.61              |
| 1:2:1592:A:H2'     | 1:2:1593:A:C8      | 2.34                     | 0.61              |
| 1:2:1665:U:O4      | 86:2:2137:OHX:N4   | 2.32                     | 0.61              |
| 27:D5:43:ASP:O     | 27:D5:45:GLU:N     | 2.33                     | 0.61              |
| 40:L3:211:GLN:NE2  | 40:L3:283:TYR:O    | 2.33                     | 0.61              |
| 44:L7:121:LYS:HB2  | 57:N1:133:ALA:HB3  | 1.81                     | 0.61              |
| 48:M1:15:GLU:HB3   | 48:M1:130:VAL:HG22 | 1.82                     | 0.61              |
| 55:M9:86:GLU:OE2   | 55:M9:91:SER:N     | 2.30                     | 0.61              |
| 1:6:820:U:O2'      | 1:6:821:U:H5''     | 2.00                     | 0.61              |
| 5:s3:105:MET:HG2   | 5:s3:122:VAL:HG21  | 1.82                     | 0.61              |
| 86:7:218:OHX:N1    | 86:7:226:OHX:N2    | 2.49                     | 0.61              |
| 52:m6:108:ILE:HG12 | 52:m6:108:ILE:O    | 1.99                     | 0.61              |
| 62:n6:120:GLN:OE1  | 62:n6:126:LEU:HA   | 2.00                     | 0.61              |
| 82:p0:40:GLU:OE2   | 82:p0:104:ARG:NE   | 2.33                     | 0.61              |
| 1:2:569:C:H41      | 25:D3:69:ARG:HH12  | 1.48                     | 0.61              |
| 1:2:1280:C:H2'     | 1:2:1281:G:H8      | 1.66                     | 0.61              |
| 11:S9:17:ARG:O     | 11:S9:23:ARG:NH2   | 2.33                     | 0.61              |
| 19:C7:20:TYR:CE1   | 19:C7:38:ILE:HD11  | 2.36                     | 0.61              |
| 20:C8:53:ASP:HB3   | 20:C8:56:LYS:HG3   | 1.81                     | 0.61              |
| 36:1:1524:A:OP1    | 61:N5:92:LYS:NZ    | 2.25                     | 0.61              |
| 47:M0:21:ARG:NH2   | 47:M0:22:TYR:OH    | 2.33                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:1427:A:O2'     | 1:6:1428:G:OP1     | 2.17                     | 0.61              |
| 14:c2:88:LEU:H     | 14:c2:140:PHE:HE1  | 1.48                     | 0.61              |
| 36:5:3103:A:OP2    | 86:5:4157:OHX:N4   | 2.34                     | 0.61              |
| 86:5:4020:OHX:N6   | 86:5:4215:OHX:N4   | 2.47                     | 0.61              |
| 54:m8:30:VAL:O     | 54:m8:34:THR:HG23  | 2.01                     | 0.61              |
| 1:2:143:G:N7       | 8:S6:177:ARG:NH2   | 2.48                     | 0.61              |
| 1:2:1564:U:H2'     | 1:2:1565:C:C6      | 2.35                     | 0.61              |
| 3:S1:171:ILE:HD12  | 3:S1:197:ILE:HD13  | 1.80                     | 0.61              |
| 9:S7:49:ILE:O      | 9:S7:57:ALA:N      | 2.28                     | 0.61              |
| 36:1:1472:U:H5'    | 55:M9:4:LEU:HB2    | 1.82                     | 0.61              |
| 38:4:52:A:N6       | 75:O9:27:ILE:HD13  | 2.15                     | 0.61              |
| 55:M9:8:LYS:HD2    | 55:M9:22:VAL:HG23  | 1.81                     | 0.61              |
| 61:N5:67:ILE:HD12  | 61:N5:121:LYS:HG3  | 1.82                     | 0.61              |
| 7:s5:158:GLN:HG2   | 30:d8:66:LEU:HD11  | 1.83                     | 0.61              |
| 36:5:136:G:H5'     | 71:o5:95:PHE:CG    | 2.36                     | 0.61              |
| 36:5:213:A:H5''    | 62:n6:2:ALA:N      | 2.14                     | 0.61              |
| 36:5:438:A:H2'     | 36:5:494:G:H21     | 1.64                     | 0.61              |
| 36:5:1152:G:N2     | 36:5:1200:A:H61    | 1.97                     | 0.61              |
| 36:5:2407:C:H2'    | 36:5:2408:U:C6     | 2.34                     | 0.61              |
| 48:m1:54:VAL:HG13  | 48:m1:59:ILE:HD11  | 1.81                     | 0.61              |
| 53:m7:155:GLU:N    | 53:m7:155:GLU:OE2  | 2.29                     | 0.61              |
| 71:o5:101:THR:HG22 | 71:o5:104:GLN:HB2  | 1.81                     | 0.61              |
| 79:q3:73:THR:HG22  | 79:q3:76:ALA:H     | 1.65                     | 0.61              |
| 1:2:717:C:H42      | 1:2:720:G:H22      | 1.48                     | 0.61              |
| 1:2:843:U:H2'      | 1:2:844:A:H8       | 1.65                     | 0.61              |
| 1:2:1073:G:H2'     | 1:2:1074:G:H5''    | 1.83                     | 0.61              |
| 10:S8:39:GLY:HA2   | 10:S8:61:GLU:HB3   | 1.82                     | 0.61              |
| 13:C1:6:THR:O      | 13:C1:8:GLN:N      | 2.32                     | 0.61              |
| 45:L8:225:LYS:O    | 45:L8:229:VAL:HG23 | 2.00                     | 0.61              |
| 48:M1:90:GLN:HG2   | 48:M1:170:ASP:HB2  | 1.83                     | 0.61              |
| 1:6:986:G:OP2      | 86:6:2120:OHX:N2   | 2.33                     | 0.61              |
| 1:6:1524:A:H2'     | 1:6:1525:A:C8      | 2.36                     | 0.61              |
| 34:sR:170:ILE:HG13 | 34:sR:202:LEU:HD21 | 1.83                     | 0.61              |
| 36:5:1355:A:H1'    | 36:5:1356:U:OP2    | 1.99                     | 0.61              |
| 36:5:1818:U:H2'    | 36:5:1819:U:H6     | 1.64                     | 0.61              |
| 36:5:2403:G:H22    | 36:5:2404:A:H62    | 1.49                     | 0.61              |
| 39:l2:56:ALA:HB2   | 39:l2:130:SER:HB3  | 1.81                     | 0.61              |
| 40:l3:346:THR:O    | 40:l3:348:ARG:N    | 2.34                     | 0.61              |
| 1:2:1207:C:N4      | 1:2:1456:C:H5      | 1.99                     | 0.61              |
| 16:C4:30:VAL:HG22  | 16:C4:39:ILE:HG13  | 1.83                     | 0.61              |
| 24:D2:30:SER:HA    | 24:D2:34:ILE:HD12  | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1638:A:H5''   | 36:5:1639:C:OP2    | 2.00                     | 0.61              |
| 40:13:103:THR:HG21 | 40:13:147:GLU:OE2  | 2.01                     | 0.61              |
| 3:S1:206:PRO:O     | 3:S1:207:LEU:HB2   | 1.98                     | 0.61              |
| 34:SR:300:THR:HG23 | 34:SR:314:GLN:HG3  | 1.82                     | 0.61              |
| 36:1:2341:A:OP2    | 40:L3:247:ARG:NH2  | 2.34                     | 0.61              |
| 41:L4:5:GLN:HA     | 41:L4:20:LEU:O     | 2.01                     | 0.61              |
| 74:O8:45:VAL:HG23  | 74:O8:52:TYR:HB2   | 1.81                     | 0.61              |
| 1:6:191:C:O2'      | 1:6:192:U:O5'      | 2.19                     | 0.61              |
| 1:6:417:A:H4'      | 1:6:418:G:O5'      | 2.01                     | 0.61              |
| 1:6:819:G:O2'      | 1:6:821:U:OP2      | 2.19                     | 0.61              |
| 1:6:1209:C:H5''    | 33:e1:77:GLY:HA3   | 1.83                     | 0.61              |
| 1:6:1462:G:N7      | 20:c8:143:ARG:NH2  | 2.48                     | 0.61              |
| 2:s0:84:ARG:HH21   | 2:s0:201:LEU:HD12  | 1.66                     | 0.61              |
| 3:s1:71:ALA:HB3    | 16:c4:114:ARG:HH12 | 1.66                     | 0.61              |
| 18:c6:47:LYS:HZ1   | 18:c6:114:ARG:HD3  | 1.65                     | 0.61              |
| 35:sM:48:ARG:HB3   | 35:sM:50:ASN:H     | 1.65                     | 0.61              |
| 42:l5:268:GLU:O    | 42:l5:270:LYS:N    | 2.34                     | 0.61              |
| 51:m5:168:GLY:O    | 51:m5:172:ARG:HB2  | 2.00                     | 0.61              |
| 54:m8:177:GLY:O    | 54:m8:186:VAL:N    | 2.34                     | 0.61              |
| 73:o7:62:GLY:O     | 86:o7:502:OHX:N3   | 2.34                     | 0.61              |
| 1:2:1239:U:O4      | 86:2:2048:OHX:N2   | 2.34                     | 0.61              |
| 15:C3:84:ILE:HG22  | 15:C3:135:LEU:HD21 | 1.83                     | 0.61              |
| 21:C9:4:VAL:HG11   | 21:C9:137:ALA:HB2  | 1.83                     | 0.61              |
| 27:D5:59:TYR:HD2   | 27:D5:60:VAL:N     | 1.99                     | 0.61              |
| 36:1:1334:U:O2'    | 44:L7:151:ARG:NH2  | 2.31                     | 0.61              |
| 36:1:3317:U:H4'    | 36:1:3318:G:O5'    | 2.01                     | 0.61              |
| 40:L3:70:ARG:HH22  | 59:N3:120:LYS:HE3  | 1.66                     | 0.61              |
| 54:M8:161:LYS:O    | 54:M8:162:ALA:HB3  | 2.01                     | 0.61              |
| 57:N1:91:LEU:HD12  | 57:N1:96:ILE:HD11  | 1.83                     | 0.61              |
| 5:s3:75:LYS:HB3    | 12:c0:22:VAL:HG22  | 1.82                     | 0.61              |
| 6:s4:151:ASP:OD1   | 8:s6:215:ARG:NH1   | 2.33                     | 0.61              |
| 36:5:1888:U:OP1    | 40:l3:247:ARG:HD3  | 2.01                     | 0.61              |
| 41:l4:295:ILE:O    | 41:l4:299:ILE:HG12 | 2.00                     | 0.61              |
| 42:l5:76:ALA:HB3   | 42:l5:109:THR:HG22 | 1.81                     | 0.61              |
| 63:n7:23:VAL:HG12  | 63:n7:45:GLY:HA3   | 1.83                     | 0.61              |
| 70:o4:7:PHE:HD1    | 70:o4:20:ILE:HD12  | 1.66                     | 0.61              |
| 78:q2:77:CYS:SG    | 78:q2:79:THR:HG23  | 2.41                     | 0.61              |
| 1:2:839:U:H2'      | 1:2:840:U:H5'      | 1.83                     | 0.60              |
| 2:S0:121:VAL:HG23  | 2:S0:141:ILE:HG21  | 1.81                     | 0.60              |
| 24:D2:27:ILE:HD11  | 24:D2:61:ILE:HD12  | 1.82                     | 0.60              |
| 28:D6:24:VAL:HG21  | 28:D6:71:LEU:HD12  | 1.83                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1806:A:OP2    | 86:1:3986:OHX:N4   | 2.34                     | 0.60              |
| 36:1:1854:C:OP2    | 86:1:4037:OHX:N5   | 2.33                     | 0.60              |
| 36:1:2535:A:H61    | 36:1:2544:U:H3     | 1.48                     | 0.60              |
| 36:1:3078:U:H4'    | 36:1:3079:U:O5'    | 1.96                     | 0.60              |
| 53:M7:32:THR:HG21  | 53:M7:87:SER:HB3   | 1.82                     | 0.60              |
| 53:M7:67:ILE:HD12  | 53:M7:82:ARG:CZ    | 2.30                     | 0.60              |
| 73:O7:5:THR:HA     | 73:O7:8:PHE:CD2    | 2.36                     | 0.60              |
| 1:6:584:C:H1'      | 80:e0:18:THR:HG21  | 1.82                     | 0.60              |
| 28:d6:11:ASN:ND2   | 28:d6:11:ASN:O     | 2.34                     | 0.60              |
| 36:5:1815:U:O2'    | 36:5:1816:A:OP2    | 2.16                     | 0.60              |
| 40:l3:47:LEU:HG    | 40:l3:335:ILE:HD11 | 1.82                     | 0.60              |
| 40:l3:299:ASP:OD1  | 40:l3:301:THR:HG23 | 2.01                     | 0.60              |
| 44:l7:102:VAL:HG12 | 44:l7:130:ILE:HD12 | 1.83                     | 0.60              |
| 54:m8:34:THR:HG22  | 54:m8:49:LEU:HD21  | 1.82                     | 0.60              |
| 1:2:499:U:O2'      | 1:2:500:C:H5''     | 2.01                     | 0.60              |
| 12:C0:50:THR:HG22  | 12:C0:55:VAL:HG22  | 1.83                     | 0.60              |
| 26:D4:36:SER:O     | 26:D4:40:LEU:HG    | 2.01                     | 0.60              |
| 34:SR:238:ASP:N    | 34:SR:238:ASP:OD1  | 2.33                     | 0.60              |
| 38:4:79:A:H2'      | 38:4:80:A:H1'      | 1.82                     | 0.60              |
| 64:N8:6:THR:HG22   | 64:N8:9:ARG:HG2    | 1.84                     | 0.60              |
| 66:O0:26:GLY:O     | 66:O0:30:THR:HG23  | 2.01                     | 0.60              |
| 6:s4:77:ARG:HD2    | 6:s4:82:TYR:CE1    | 2.36                     | 0.60              |
| 6:s4:251:GLU:O     | 6:s4:255:ARG:HG2   | 2.01                     | 0.60              |
| 19:c7:28:PHE:HA    | 19:c7:55:THR:HG21  | 1.82                     | 0.60              |
| 36:5:1064:A:N6     | 36:5:1096:U:H3     | 1.99                     | 0.60              |
| 47:m0:156:ARG:HD3  | 47:m0:163:GLN:O    | 2.01                     | 0.60              |
| 59:n3:87:ARG:HH22  | 59:n3:137:VAL:CG2  | 2.13                     | 0.60              |
| 1:2:116:U:H2'      | 1:2:117:U:C6       | 2.37                     | 0.60              |
| 1:2:1290:U:H2'     | 1:2:1291:G:C8      | 2.36                     | 0.60              |
| 1:2:1460:A:O2'     | 35:SM:72:ARG:NH2   | 2.34                     | 0.60              |
| 25:D3:127:VAL:O    | 25:D3:130:VAL:HG22 | 2.01                     | 0.60              |
| 26:D4:83:LYS:HE2   | 26:D4:96:LEU:HB3   | 1.84                     | 0.60              |
| 36:1:1924:U:OP1    | 77:Q1:25:LYS:NZ    | 2.34                     | 0.60              |
| 36:1:2278:C:OP1    | 86:1:3961:OHX:N3   | 2.35                     | 0.60              |
| 36:1:2683:U:H2'    | 36:1:2684:C:C6     | 2.36                     | 0.60              |
| 86:1:4007:OHX:N3   | 86:1:4175:OHX:N3   | 2.50                     | 0.60              |
| 49:M3:180:ARG:HD3  | 72:O6:11:LEU:HD21  | 1.83                     | 0.60              |
| 55:M9:101:VAL:HG13 | 55:M9:104:ARG:NH1  | 2.15                     | 0.60              |
| 67:O1:54:GLU:OE2   | 67:O1:54:GLU:N     | 2.29                     | 0.60              |
| 1:6:1695:G:H21     | 1:6:1706:C:N4      | 1.99                     | 0.60              |
| 4:s2:234:PRO:O     | 4:s2:235:LEU:HB2   | 2.01                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:sM:64:LYS:O     | 35:sM:66:ALA:N     | 2.34                     | 0.60              |
| 36:5:510:G:O6      | 86:5:4023:OHX:N2   | 2.34                     | 0.60              |
| 36:5:3049:A:H5'    | 36:5:3049:A:H8     | 1.66                     | 0.60              |
| 56:n0:13:ARG:HH11  | 56:n0:13:ARG:HG3   | 1.64                     | 0.60              |
| 1:2:1428:G:H5'     | 1:2:1428:G:C8      | 2.35                     | 0.60              |
| 36:1:3050:U:OP2    | 86:1:4184:OHX:N4   | 2.35                     | 0.60              |
| 36:1:3066:U:O4     | 86:1:4138:OHX:N5   | 2.34                     | 0.60              |
| 86:1:3962:OHX:N6   | 44:L7:217:PRO:O    | 2.34                     | 0.60              |
| 37:3:4:U:H2'       | 37:3:5:G:C8        | 2.36                     | 0.60              |
| 53:M7:33:ALA:HB1   | 53:M7:117:ILE:HG12 | 1.84                     | 0.60              |
| 56:N0:155:ARG:NH2  | 56:N0:171:PHE:O    | 2.35                     | 0.60              |
| 24:d2:114:GLU:HG2  | 24:d2:118:ARG:HH21 | 1.66                     | 0.60              |
| 36:5:1717:U:H2'    | 36:5:1718:G:C8     | 2.37                     | 0.60              |
| 2:S0:188:LEU:HD12  | 2:S0:189:VAL:HG12  | 1.83                     | 0.60              |
| 7:S5:163:SER:HB2   | 30:D8:48:VAL:HG23  | 1.83                     | 0.60              |
| 21:C9:32:GLY:H     | 21:C9:34:VAL:HG12  | 1.67                     | 0.60              |
| 34:SR:211:ILE:HG22 | 34:SR:223:TRP:HD1  | 1.66                     | 0.60              |
| 36:1:3218:A:H5''   | 36:1:3219:G:C5     | 2.37                     | 0.60              |
| 41:L4:33:ASP:O     | 41:L4:37:THR:HG23  | 2.00                     | 0.60              |
| 54:M8:170:ARG:O    | 54:M8:171:LYS:HB3  | 2.00                     | 0.60              |
| 69:O3:75:HIS:HB3   | 69:O3:80:VAL:HG12  | 1.83                     | 0.60              |
| 1:6:874:C:H2'      | 1:6:875:G:C8       | 2.37                     | 0.60              |
| 1:6:1250:U:O2      | 33:e1:135:HIS:ND1  | 2.34                     | 0.60              |
| 1:6:1508:U:O4      | 86:6:2055:OHX:N4   | 2.34                     | 0.60              |
| 36:5:1103:A:H3'    | 36:5:1104:G:H5'    | 1.83                     | 0.60              |
| 36:5:1716:U:H6     | 36:5:1716:U:H5'    | 1.67                     | 0.60              |
| 36:5:3122:A:N1     | 46:l9:70:THR:HG21  | 2.16                     | 0.60              |
| 1:2:1067:C:H2'     | 1:2:1068:C:H6      | 1.65                     | 0.60              |
| 1:2:1338:C:H1'     | 1:2:1410:A:C4      | 2.37                     | 0.60              |
| 1:2:1769:U:OP2     | 86:2:2146:OHX:N1   | 2.34                     | 0.60              |
| 4:S2:226:THR:OG1   | 4:S2:228:ASN:OD1   | 2.19                     | 0.60              |
| 36:1:1764:U:H5''   | 55:M9:43:LYS:HE2   | 1.84                     | 0.60              |
| 40:L3:347:SER:HB3  | 40:L3:350:ALA:H    | 1.65                     | 0.60              |
| 44:L7:47:ARG:NH1   | 44:L7:183:ASP:OD2  | 2.35                     | 0.60              |
| 5:s3:40:ARG:HG3    | 22:d0:110:PRO:HB3  | 1.84                     | 0.60              |
| 34:sR:216:LYS:HA   | 34:sR:239:GLU:HG3  | 1.83                     | 0.60              |
| 86:5:4001:OHX:N4   | 86:5:4090:OHX:N2   | 2.49                     | 0.60              |
| 86:8:215:OHX:N2    | 86:8:223:OHX:N1    | 2.48                     | 0.60              |
| 39:l2:230:VAL:O    | 39:l2:233:GLN:HB2  | 2.01                     | 0.60              |
| 45:l8:133:LYS:HB2  | 45:l8:199:ALA:O    | 2.02                     | 0.60              |
| 36:1:1176:C:H2'    | 36:1:1177:G:N2     | 2.17                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1278:A:O2'    | 36:1:1279:C:O5'    | 2.19                     | 0.60              |
| 36:1:1609:C:H5''   | 61:N5:125:ARG:HH11 | 1.67                     | 0.60              |
| 36:1:2736:A:OP1    | 57:N1:92:ARG:NH1   | 2.34                     | 0.60              |
| 56:N0:166:LYS:O    | 56:N0:167:ARG:HB2  | 2.01                     | 0.60              |
| 1:6:474:A:OP1      | 11:s9:145:SER:OG   | 2.15                     | 0.60              |
| 1:6:523:G:H5'      | 26:d4:60:PHE:O     | 2.02                     | 0.60              |
| 1:6:1081:A:H1'     | 1:6:1082:C:H5      | 1.67                     | 0.60              |
| 36:5:2514:U:H6     | 36:5:2514:U:OP1    | 1.85                     | 0.60              |
| 36:5:2569:A:H4'    | 36:5:2570:U:H5'    | 1.84                     | 0.60              |
| 48:m1:155:THR:O    | 48:m1:159:THR:HG23 | 2.02                     | 0.60              |
| 62:n6:37:LYS:H     | 62:n6:37:LYS:HE2   | 1.64                     | 0.60              |
| 1:2:1542:G:N2      | 1:2:1568:C:H1'     | 2.16                     | 0.60              |
| 10:S8:188:GLU:OE2  | 13:C1:15:LYS:NZ    | 2.29                     | 0.60              |
| 17:C5:18:ARG:NH1   | 20:C8:90:ASN:O     | 2.34                     | 0.60              |
| 36:1:381:U:O4      | 86:1:4065:OHX:N4   | 2.34                     | 0.60              |
| 36:1:1599:G:OP1    | 86:1:4088:OHX:N5   | 2.35                     | 0.60              |
| 36:1:1615:C:OP1    | 86:1:4182:OHX:N3   | 2.35                     | 0.60              |
| 36:1:3329:U:H5''   | 40:L3:308:MET:HE3  | 1.84                     | 0.60              |
| 39:L2:202:VAL:HG13 | 39:L2:217:GLN:HB3  | 1.83                     | 0.60              |
| 42:L5:107:ARG:HH22 | 42:L5:120:LYS:HA   | 1.66                     | 0.60              |
| 63:N7:87:LEU:HB2   | 63:N7:127:ASN:ND2  | 2.15                     | 0.60              |
| 1:6:716:C:H42      | 1:6:722:G:H1       | 1.50                     | 0.60              |
| 1:6:1672:G:H2'     | 1:6:1673:G:C8      | 2.37                     | 0.60              |
| 1:6:1766:A:H5''    | 86:6:2126:OHX:N3   | 2.16                     | 0.60              |
| 25:d3:51:GLY:O     | 25:d3:101:GLU:HA   | 2.02                     | 0.60              |
| 36:5:1804:A:H2'    | 36:5:1805:C:H6     | 1.65                     | 0.60              |
| 36:5:2103:U:OP1    | 55:m9:88:ARG:NH1   | 2.34                     | 0.60              |
| 41:l4:16:THR:HG22  | 41:l4:18:ASN:N     | 2.14                     | 0.60              |
| 44:l7:228:SER:HA   | 44:l7:232:ARG:HH21 | 1.66                     | 0.60              |
| 51:m5:68:ARG:HA    | 51:m5:98:LEU:HD21  | 1.82                     | 0.60              |
| 1:2:4:C:O2'        | 11:S9:17:ARG:NH1   | 2.35                     | 0.60              |
| 1:2:514:G:N1       | 1:2:543:C:H5       | 2.00                     | 0.60              |
| 1:2:1280:C:H2'     | 1:2:1281:G:C8      | 2.36                     | 0.60              |
| 8:S6:57:ASP:OD1    | 8:S6:72:ARG:NH1    | 2.35                     | 0.60              |
| 10:S8:8:ARG:NH2    | 10:S8:19:ALA:O     | 2.34                     | 0.60              |
| 36:1:1934:G:N7     | 86:1:3888:OHX:N2   | 2.50                     | 0.60              |
| 41:L4:20:LEU:HD11  | 41:L4:252:GLU:HG3  | 1.84                     | 0.60              |
| 41:L4:98:ARG:HD2   | 41:L4:99:MET:O     | 2.02                     | 0.60              |
| 55:M9:23:TRP:CZ3   | 55:M9:25:ASP:HB2   | 2.37                     | 0.60              |
| 64:N8:116:GLY:HA2  | 64:N8:137:LYS:NZ   | 2.17                     | 0.60              |
| 1:6:489:C:O2'      | 1:6:490:C:O4'      | 2.19                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:1402:G:H5'     | 19:c7:4:VAL:HG22   | 1.83                     | 0.60              |
| 3:s1:103:MET:HB3   | 3:s1:215:VAL:HG12  | 1.83                     | 0.60              |
| 4:s2:70:ASP:OD1    | 4:s2:133:LYS:NZ    | 2.28                     | 0.60              |
| 6:s4:126:VAL:HG13  | 6:s4:158:ASP:O     | 2.01                     | 0.60              |
| 20:c8:140:THR:HA   | 20:c8:143:ARG:NH1  | 2.17                     | 0.60              |
| 36:5:223:U:O4      | 86:5:4242:OHX:N4   | 2.34                     | 0.60              |
| 36:5:955:U:H2'     | 36:5:956:U:C6      | 2.37                     | 0.60              |
| 36:5:1493:G:O6     | 75:o9:2:ALA:N      | 2.34                     | 0.60              |
| 39:l2:112:ILE:HD11 | 39:l2:168:VAL:HG12 | 1.83                     | 0.60              |
| 42:l5:120:LYS:HD3  | 42:l5:123:GLU:OE1  | 2.02                     | 0.60              |
| 49:m3:37:ASN:O     | 49:m3:41:THR:HG23  | 2.01                     | 0.60              |
| 77:q1:9:ARG:HG3    | 77:q1:9:ARG:NH1    | 2.15                     | 0.60              |
| 1:2:851:U:H2'      | 1:2:852:C:C6       | 2.37                     | 0.60              |
| 25:D3:130:VAL:O    | 25:D3:131:SER:HB3  | 2.02                     | 0.60              |
| 26:D4:62:THR:HA    | 26:D4:69:SER:HA    | 1.84                     | 0.60              |
| 36:1:776:U:C5      | 36:1:2719:U:O2     | 2.53                     | 0.60              |
| 36:1:3113:A:OP1    | 46:L9:73:SER:OG    | 2.19                     | 0.60              |
| 40:L3:169:THR:HG21 | 40:L3:171:LEU:HD12 | 1.84                     | 0.60              |
| 41:L4:36:HIS:O     | 41:L4:40:THR:HG23  | 2.00                     | 0.60              |
| 59:N3:74:MET:HE3   | 59:N3:102:ILE:HB   | 1.82                     | 0.60              |
| 1:6:697:C:OP2      | 86:6:2074:OHX:N5   | 2.35                     | 0.60              |
| 36:5:2433:U:H1'    | 51:m5:125:SER:HB3  | 1.82                     | 0.60              |
| 36:5:3214:U:C4     | 50:m4:121:MET:HG3  | 2.36                     | 0.60              |
| 40:l3:303:LYS:HZ2  | 40:l3:361:THR:HB   | 1.66                     | 0.60              |
| 76:q0:78:ILE:HD11  | 76:q0:83:LYS:HA    | 1.82                     | 0.60              |
| 1:2:1477:G:H2'     | 1:2:1478:G:C8      | 2.37                     | 0.59              |
| 23:D1:71:ARG:HG3   | 23:D1:83:TRP:CH2   | 2.37                     | 0.59              |
| 36:1:2799:A:H1'    | 64:N8:42:ARG:NH2   | 2.16                     | 0.59              |
| 36:1:2818:U:H5'    | 36:1:2818:U:C6     | 2.37                     | 0.59              |
| 36:1:3103:A:OP2    | 86:1:4170:OHX:N1   | 2.35                     | 0.59              |
| 40:L3:81:THR:O     | 40:L3:81:THR:HG22  | 2.02                     | 0.59              |
| 45:L8:163:VAL:HG22 | 45:L8:166:LEU:HD12 | 1.84                     | 0.59              |
| 53:M7:129:THR:HG23 | 53:M7:139:TYR:HB2  | 1.84                     | 0.59              |
| 63:N7:21:LYS:HG2   | 63:N7:46:ILE:O     | 2.03                     | 0.59              |
| 1:6:1688:U:H2'     | 1:6:1689:A:C8      | 2.37                     | 0.59              |
| 20:c8:145:ARG:HD3  | 35:sM:68:ARG:CZ    | 2.32                     | 0.59              |
| 36:5:385:A:H2'     | 36:5:386:A:C8      | 2.37                     | 0.59              |
| 36:5:2138:A:HO2'   | 73:o7:2:GLY:N      | 2.00                     | 0.59              |
| 36:5:2988:C:P      | 52:m6:68:ARG:NH1   | 2.74                     | 0.59              |
| 37:7:67:G:H5'      | 42:l5:10:SER:HB2   | 1.83                     | 0.59              |
| 41:l4:144:LYS:O    | 86:l4:402:OHX:N1   | 2.34                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:m1:24:GLY:HA2   | 48:m1:65:ILE:HG23  | 1.84                     | 0.59              |
| 49:m3:133:PRO:O    | 49:m3:135:ALA:N    | 2.35                     | 0.59              |
| 53:m7:64:ASN:O     | 53:m7:67:ILE:HG12  | 2.02                     | 0.59              |
| 56:n0:91:TYR:O     | 56:n0:137:ARG:NH1  | 2.35                     | 0.59              |
| 1:2:1358:G:H2'     | 1:2:1359:C:C6      | 2.38                     | 0.59              |
| 4:S2:56:ILE:HG23   | 4:S2:61:LEU:HB2    | 1.84                     | 0.59              |
| 10:S8:116:HIS:O    | 10:S8:146:ARG:NH1  | 2.35                     | 0.59              |
| 34:SR:255:ALA:HB2  | 34:SR:292:LEU:HD22 | 1.85                     | 0.59              |
| 36:1:2518:C:OP1    | 86:1:4209:OHX:N5   | 2.35                     | 0.59              |
| 41:L4:145:ILE:O    | 86:L4:404:OHX:N5   | 2.35                     | 0.59              |
| 42:L5:105:ILE:O    | 42:L5:109:THR:HG23 | 2.02                     | 0.59              |
| 52:M6:42:ASN:OD1   | 52:M6:125:ARG:HD3  | 2.02                     | 0.59              |
| 75:O9:5:LYS:HE3    | 75:O9:13:MET:HE1   | 1.84                     | 0.59              |
| 1:6:152:U:C2       | 1:6:163:G:N2       | 2.70                     | 0.59              |
| 36:5:2528:G:N7     | 86:5:4206:OHX:N3   | 2.50                     | 0.59              |
| 36:5:2717:U:OP1    | 86:5:4068:OHX:N3   | 2.35                     | 0.59              |
| 48:m1:101:ASN:HB3  | 48:m1:130:VAL:HA   | 1.83                     | 0.59              |
| 49:m3:42:ARG:O     | 49:m3:46:ILE:HG12  | 2.02                     | 0.59              |
| 72:o6:63:ASN:O     | 72:o6:65:GLY:N     | 2.35                     | 0.59              |
| 6:S4:73:ASP:OD2    | 6:S4:122:LYS:NZ    | 2.24                     | 0.59              |
| 36:1:2223:A:OP2    | 36:1:2223:A:H8     | 1.84                     | 0.59              |
| 37:3:17:A:OP1      | 42:L5:2:ALA:N      | 2.34                     | 0.59              |
| 70:O4:44:CYS:SG    | 70:O4:81:CYS:HB3   | 2.42                     | 0.59              |
| 74:O8:8:ILE:H      | 74:O8:8:ILE:HD12   | 1.67                     | 0.59              |
| 1:6:75:U:O2'       | 1:6:76:A:O4'       | 2.20                     | 0.59              |
| 1:6:500:C:O2'      | 1:6:501:U:O4'      | 2.21                     | 0.59              |
| 1:6:1183:A:C4      | 17:c5:100:LYS:HD3  | 2.37                     | 0.59              |
| 1:6:1697:G:H8      | 1:6:1705:C:N3      | 2.00                     | 0.59              |
| 6:s4:121:TYR:HA    | 6:s4:163:ASP:O     | 2.02                     | 0.59              |
| 22:d0:28:SER:HB3   | 22:d0:34:LEU:HD12  | 1.84                     | 0.59              |
| 39:l2:27:ALA:O     | 39:l2:128:ARG:NH2  | 2.35                     | 0.59              |
| 40:l3:4:ARG:HG3    | 40:l3:4:ARG:HH11   | 1.65                     | 0.59              |
| 47:m0:72:ALA:O     | 47:m0:76:MET:HG2   | 2.02                     | 0.59              |
| 55:m9:106:LEU:HD13 | 55:m9:138:LEU:HD11 | 1.84                     | 0.59              |
| 1:2:482:U:H2'      | 1:2:483:A:H8       | 1.66                     | 0.59              |
| 1:2:530:C:O2       | 26:D4:61:ARG:NH2   | 2.36                     | 0.59              |
| 1:2:539:G:OP2      | 1:2:539:G:H8       | 1.86                     | 0.59              |
| 1:2:843:U:H2'      | 1:2:844:A:C8       | 2.38                     | 0.59              |
| 1:2:1657:U:O4      | 86:2:2090:OHX:N4   | 2.36                     | 0.59              |
| 12:C0:46:LEU:O     | 12:C0:50:THR:HG23  | 2.02                     | 0.59              |
| 36:1:1383:G:O3'    | 41:L4:138:ARG:NH2  | 2.36                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:2107:A:C2     | 36:1:3344:A:H8     | 2.19                     | 0.59              |
| 40:L3:77:THR:HG23  | 40:L3:326:GLY:O    | 2.02                     | 0.59              |
| 17:c5:68:PRO:O     | 86:c5:201:OHX:N1   | 2.35                     | 0.59              |
| 17:c5:126:VAL:O    | 17:c5:127:ARG:HB2  | 2.02                     | 0.59              |
| 20:c8:26:ILE:HD11  | 20:c8:31:ALA:HA    | 1.83                     | 0.59              |
| 36:5:330:G:OP2     | 86:5:4049:OHX:N1   | 2.35                     | 0.59              |
| 36:5:1178:G:H5'    | 69:o3:18:ARG:HD3   | 1.84                     | 0.59              |
| 43:l6:50:LYS:HG2   | 43:l6:74:VAL:CG2   | 2.33                     | 0.59              |
| 46:l9:57:VAL:HG23  | 46:l9:68:LEU:HG    | 1.85                     | 0.59              |
| 56:n0:81:TYR:CE1   | 56:n0:90:MET:HE3   | 2.38                     | 0.59              |
| 1:2:876:G:H1'      | 1:2:944:A:O4'      | 2.02                     | 0.59              |
| 2:S0:56:LYS:NZ     | 23:D1:66:ASP:OD1   | 2.31                     | 0.59              |
| 19:C7:27:ASP:OD2   | 19:C7:30:THR:HG22  | 2.01                     | 0.59              |
| 19:C7:50:ILE:O     | 19:C7:54:THR:HG23  | 2.02                     | 0.59              |
| 21:C9:52:GLY:HA2   | 21:C9:55:TYR:CD2   | 2.37                     | 0.59              |
| 86:1:3943:OHX:N1   | 86:1:4200:OHX:N4   | 2.50                     | 0.59              |
| 41:L4:354:VAL:HG11 | 57:N1:143:THR:HG21 | 1.83                     | 0.59              |
| 47:M0:210:ILE:HA   | 47:M0:217:PHE:HE2  | 1.68                     | 0.59              |
| 56:N0:82:ASP:OD1   | 56:N0:87:THR:HB    | 2.02                     | 0.59              |
| 63:N7:14:VAL:HG13  | 70:O4:86:LYS:HG2   | 1.83                     | 0.59              |
| 1:6:918:U:H2'      | 1:6:919:A:H8       | 1.68                     | 0.59              |
| 1:6:1207:C:H42     | 1:6:1456:C:H5      | 1.50                     | 0.59              |
| 14:c2:81:ASP:O     | 14:c2:83:GLU:N     | 2.35                     | 0.59              |
| 18:c6:47:LYS:NZ    | 18:c6:114:ARG:HD3  | 2.16                     | 0.59              |
| 26:d4:122:GLY:HA2  | 26:d4:125:LEU:HB3  | 1.85                     | 0.59              |
| 36:5:1235:U:H4'    | 36:5:1236:G:H5'    | 1.83                     | 0.59              |
| 36:5:2401:A:H1'    | 41:l4:68:GLY:O     | 2.02                     | 0.59              |
| 36:5:2977:G:OP1    | 86:5:4151:OHX:N4   | 2.36                     | 0.59              |
| 86:5:4020:OHX:N5   | 86:5:4215:OHX:N1   | 2.49                     | 0.59              |
| 38:8:43:A:OP1      | 86:8:224:OHX:N3    | 2.35                     | 0.59              |
| 41:l4:191:LYS:HG3  | 41:l4:194:TYR:CZ   | 2.37                     | 0.59              |
| 1:2:1429:G:C1'     | 22:D0:74:GLU:HG2   | 2.31                     | 0.59              |
| 10:S8:138:ASN:N    | 10:S8:138:ASN:OD1  | 2.36                     | 0.59              |
| 21:C9:30:VAL:HG12  | 21:C9:54:PHE:CD2   | 2.37                     | 0.59              |
| 36:1:3242:G:N2     | 36:1:3245:A:H5''   | 2.18                     | 0.59              |
| 86:1:3976:OHX:N3   | 86:1:4159:OHX:N1   | 2.51                     | 0.59              |
| 52:M6:78:ARG:HH11  | 52:M6:78:ARG:HG2   | 1.68                     | 0.59              |
| 10:s8:8:ARG:CZ     | 10:s8:22:ARG:HE    | 2.16                     | 0.59              |
| 26:d4:122:GLY:O    | 26:d4:126:ALA:N    | 2.32                     | 0.59              |
| 27:d5:47:TYR:CZ    | 27:d5:51:LEU:HD11  | 2.38                     | 0.59              |
| 36:5:1586:G:OP1    | 86:5:3991:OHX:N3   | 2.36                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:5:1877:U:H5''   | 36:5:1878:G:H5'   | 1.83                     | 0.59              |
| 36:5:2810:C:OP1    | 86:5:4079:OHX:N3  | 2.36                     | 0.59              |
| 1:2:280:U:O2'      | 1:2:281:G:OP2     | 2.17                     | 0.59              |
| 1:2:1619:C:H1'     | 30:D8:22:ARG:HH21 | 1.67                     | 0.59              |
| 1:2:1657:U:C4      | 86:2:2090:OHX:N2  | 2.70                     | 0.59              |
| 2:S0:26:ALA:HB3    | 2:S0:149:LEU:HB2  | 1.84                     | 0.59              |
| 3:S1:85:LYS:HB3    | 3:S1:101:HIS:HB3  | 1.84                     | 0.59              |
| 7:S5:43:PHE:HZ     | 7:S5:90:ILE:HG21  | 1.66                     | 0.59              |
| 21:C9:52:GLY:HA2   | 21:C9:55:TYR:HD2  | 1.68                     | 0.59              |
| 36:1:1043:C:O3'    | 47:M0:90:ARG:NH1  | 2.35                     | 0.59              |
| 36:1:2443:A:N6     | 36:1:2504:U:O4    | 2.35                     | 0.59              |
| 41:L4:91:GLY:HA3   | 41:L4:93:MET:HE1  | 1.84                     | 0.59              |
| 59:N3:17:LEU:HD21  | 59:N3:98:ASN:CG   | 2.28                     | 0.59              |
| 36:5:2284:C:O2     | 86:5:4177:OHX:N1  | 2.36                     | 0.59              |
| 46:I9:166:ARG:HH21 | 46:I9:168:ARG:NH1 | 2.00                     | 0.59              |
| 73:O7:21:ARG:HD2   | 73:O7:37:CYS:SG   | 2.42                     | 0.59              |
| 86:2:2091:OHX:N5   | 86:2:2132:OHX:N6  | 2.51                     | 0.59              |
| 15:C3:27:LYS:H     | 15:C3:27:LYS:HE2  | 1.66                     | 0.59              |
| 30:D8:12:VAL:HG22  | 30:D8:28:VAL:HG11 | 1.84                     | 0.59              |
| 41:L4:316:ASN:OD1  | 41:L4:318:LEU:HB2 | 2.03                     | 0.59              |
| 49:M3:42:ARG:O     | 49:M3:46:ILE:HB   | 2.03                     | 0.59              |
| 51:M5:38:ARG:HH11  | 51:M5:38:ARG:CG   | 2.15                     | 0.59              |
| 51:M5:96:ARG:HG2   | 51:M5:96:ARG:NH1  | 2.17                     | 0.59              |
| 60:N4:4:GLU:HG2    | 60:N4:30:ARG:CD   | 2.33                     | 0.59              |
| 70:O4:74:ARG:HG2   | 70:O4:75:ALA:N    | 2.18                     | 0.59              |
| 75:O9:48:LYS:O     | 86:O9:101:OHX:N2  | 2.35                     | 0.59              |
| 1:6:800:U:H2'      | 1:6:801:G:H8      | 1.66                     | 0.59              |
| 8:s6:162:VAL:HG21  | 8:s6:171:LYS:HD3  | 1.84                     | 0.59              |
| 13:c1:99:ARG:NH1   | 25:d3:7:ARG:O     | 2.35                     | 0.59              |
| 86:5:3978:OHX:N6   | 86:5:4196:OHX:N3  | 2.50                     | 0.59              |
| 42:I5:279:LYS:HD3  | 42:I5:282:ARG:NH2 | 2.17                     | 0.59              |
| 57:n1:135:PRO:O    | 57:n1:136:ARG:HB2 | 2.02                     | 0.59              |
| 64:n8:13:GLY:O     | 68:O2:36:LYS:HE2  | 2.02                     | 0.59              |
| 68:O2:122:PRO:O    | 68:O2:123:LYS:HB2 | 2.02                     | 0.59              |
| 2:S0:56:LYS:HD2    | 2:S0:158:VAL:HG23 | 1.83                     | 0.59              |
| 16:C4:29:HIS:HB2   | 16:C4:41:ARG:HA   | 1.85                     | 0.59              |
| 36:1:1481:A:O2'    | 36:1:1858:A:C2    | 2.49                     | 0.59              |
| 36:1:2295:A:OP1    | 59:N3:63:LYS:NZ   | 2.36                     | 0.59              |
| 4:s2:99:LYS:HG3    | 4:s2:117:THR:HG22 | 1.85                     | 0.59              |
| 80:e0:46:ASN:HD21  | 80:e0:48:THR:HG23 | 1.68                     | 0.59              |
| 33:e1:80:ARG:NH1   | 33:e1:80:ARG:HB2  | 2.18                     | 0.59              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1506:A:H1'    | 36:5:1848:G:O6     | 2.03                     | 0.59              |
| 36:5:3078:U:O2'    | 86:5:4193:OHX:N1   | 2.36                     | 0.59              |
| 36:5:3317:U:H4'    | 36:5:3318:G:O5'    | 2.03                     | 0.59              |
| 57:n1:14:MET:HE3   | 57:n1:58:GLN:CB    | 2.33                     | 0.59              |
| 60:n4:23:ARG:NH2   | 60:n4:25:ASP:OD1   | 2.23                     | 0.59              |
| 1:2:855:A:C2       | 1:2:857:U:H1'      | 2.37                     | 0.59              |
| 4:S2:98:PHE:CZ     | 35:SM:116:GLU:HG3  | 2.38                     | 0.59              |
| 8:S6:70:PRO:O      | 8:S6:98:ARG:NH1    | 2.36                     | 0.59              |
| 14:C2:52:LEU:O     | 14:C2:85:LYS:NZ    | 2.35                     | 0.59              |
| 20:C8:125:ILE:HG12 | 35:SM:61:ILE:HG23  | 1.84                     | 0.59              |
| 34:SR:13:LEU:HB2   | 34:SR:310:ILE:HB   | 1.84                     | 0.59              |
| 36:1:1845:G:H5'    | 36:1:1846:C:H5'    | 1.84                     | 0.59              |
| 36:1:2169:G:O6     | 86:M5:303:OHX:N4   | 2.35                     | 0.59              |
| 39:L2:245:LEU:HD23 | 39:L2:247:ARG:HH11 | 1.68                     | 0.59              |
| 40:L3:25:ILE:HD13  | 40:L3:25:ILE:N     | 2.18                     | 0.59              |
| 56:N0:137:ARG:HG2  | 56:N0:139:TYR:CE1  | 2.37                     | 0.59              |
| 1:6:75:U:O2'       | 1:6:76:A:O5'       | 2.21                     | 0.59              |
| 1:6:246:G:C2       | 13:c1:40:LEU:HD22  | 2.38                     | 0.59              |
| 1:6:624:G:H2'      | 1:6:625:C:H6       | 1.67                     | 0.59              |
| 21:c9:115:GLU:OE1  | 21:c9:123:ARG:NH1  | 2.35                     | 0.59              |
| 34:sR:20:VAL:HG11  | 34:sR:310:ILE:HG12 | 1.84                     | 0.59              |
| 36:5:149:U:OP2     | 51:m5:49:ARG:NH1   | 2.36                     | 0.59              |
| 36:5:1781:C:H2'    | 36:5:1782:U:C6     | 2.38                     | 0.59              |
| 38:8:83:C:H4'      | 38:8:85:G:N3       | 2.18                     | 0.59              |
| 39:l2:187:HIS:ND1  | 39:l2:190:ARG:NH1  | 2.50                     | 0.59              |
| 7:S5:110:ALA:HA    | 7:S5:113:ILE:HD12  | 1.85                     | 0.58              |
| 18:C6:47:LYS:HZ1   | 18:C6:114:ARG:HG2  | 1.67                     | 0.58              |
| 24:D2:86:ILE:HG13  | 24:D2:87:GLU:N     | 2.17                     | 0.58              |
| 30:D8:52:ASP:N     | 30:D8:52:ASP:OD1   | 2.36                     | 0.58              |
| 36:1:612:U:OP1     | 43:L6:21:THR:HB    | 2.03                     | 0.58              |
| 36:1:627:U:H2'     | 36:1:628:A:C8      | 2.38                     | 0.58              |
| 36:1:1565:G:N2     | 36:1:1574:C:O2     | 2.36                     | 0.58              |
| 36:1:3115:C:OP1    | 46:L9:62:ARG:NH2   | 2.35                     | 0.58              |
| 86:1:3943:OHX:N3   | 86:1:4200:OHX:N6   | 2.51                     | 0.58              |
| 77:Q1:6:ARG:O      | 77:Q1:10:THR:HG23  | 2.02                     | 0.58              |
| 1:6:826:U:O4       | 86:6:2066:OHX:N3   | 2.35                     | 0.58              |
| 3:s1:82:ARG:NH2    | 3:s1:188:LEU:O     | 2.36                     | 0.58              |
| 16:c4:107:ARG:HB2  | 16:c4:107:ARG:NH2  | 2.17                     | 0.58              |
| 24:d2:89:TRP:O     | 24:d2:93:LEU:HB2   | 2.03                     | 0.58              |
| 36:5:2875:U:H3     | 36:5:2952:G:H1     | 1.50                     | 0.58              |
| 60:n4:100:VAL:O    | 60:n4:104:ASN:ND2  | 2.33                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 67:o1:70:ARG:HD2  | 67:o1:102:LYS:HE2 | 1.85                     | 0.58              |
| 1:2:514:G:O2'     | 1:2:515:A:H5'     | 2.03                     | 0.58              |
| 3:S1:81:PHE:HD2   | 3:S1:82:ARG:HG3   | 1.68                     | 0.58              |
| 6:S4:194:THR:O    | 6:S4:195:ILE:HB   | 2.03                     | 0.58              |
| 16:C4:29:HIS:ND1  | 16:C4:29:HIS:O    | 2.36                     | 0.58              |
| 21:C9:61:VAL:O    | 21:C9:65:ILE:HG13 | 2.03                     | 0.58              |
| 28:D6:17:HIS:ND1  | 28:D6:18:VAL:O    | 2.36                     | 0.58              |
| 46:L9:106:LYS:H   | 46:L9:109:ALA:HB2 | 1.68                     | 0.58              |
| 49:M3:24:VAL:HG21 | 49:M3:26:PHE:CE2  | 2.38                     | 0.58              |
| 3:s1:180:THR:HG23 | 3:s1:183:GLN:OE1  | 2.02                     | 0.58              |
| 6:s4:184:THR:C    | 6:s4:189:LEU:HD13 | 2.28                     | 0.58              |
| 19:c7:6:THR:OG1   | 19:c7:8:THR:HG23  | 2.03                     | 0.58              |
| 86:5:4020:OHX:N3  | 86:5:4215:OHX:N4  | 2.51                     | 0.58              |
| 1:2:1006:C:O2     | 86:2:2146:OHX:N2  | 2.36                     | 0.58              |
| 36:1:1355:A:H5''  | 36:1:1356:U:C5    | 2.37                     | 0.58              |
| 36:1:1427:U:OP2   | 64:N8:4:ARG:NH2   | 2.26                     | 0.58              |
| 74:O8:31:LEU:HA   | 74:O8:37:PRO:HA   | 1.84                     | 0.58              |
| 1:6:1258:U:H4'    | 12:c0:2:LEU:HD22  | 1.84                     | 0.58              |
| 4:s2:170:ILE:HB   | 4:s2:197:TYR:HB2  | 1.84                     | 0.58              |
| 6:s4:73:ASP:OD2   | 6:s4:122:LYS:NZ   | 2.23                     | 0.58              |
| 36:5:173:G:HO2'   | 36:5:174:C:H6     | 1.51                     | 0.58              |
| 36:5:3049:A:H5''  | 40:l3:53:MET:HB2  | 1.84                     | 0.58              |
| 38:8:90:U:O2      | 86:8:219:OHX:N2   | 2.36                     | 0.58              |
| 41:l4:143:GLU:O   | 86:l4:402:OHX:N1  | 2.37                     | 0.58              |
| 86:2:2091:OHX:N1  | 86:2:2132:OHX:N2  | 2.52                     | 0.58              |
| 4:S2:228:ASN:ND2  | 23:D1:1:MET:HB3   | 2.17                     | 0.58              |
| 36:1:1233:G:N2    | 36:1:1255:C:N3    | 2.43                     | 0.58              |
| 36:1:1947:G:H1    | 36:1:2101:C:H42   | 1.49                     | 0.58              |
| 36:1:2514:U:H5'   | 45:L8:68:ARG:HG3  | 1.86                     | 0.58              |
| 1:6:66:U:H4'      | 1:6:67:A:OP1      | 2.03                     | 0.58              |
| 1:6:151:G:N2      | 1:6:163:G:H22     | 2.01                     | 0.58              |
| 36:5:2814:G:OP1   | 41:l4:73:ARG:NH2  | 2.34                     | 0.58              |
| 1:2:639:U:OP1     | 9:S7:117:THR:OG1  | 2.20                     | 0.58              |
| 1:2:1331:A:OP1    | 19:C7:45:ARG:NH2  | 2.37                     | 0.58              |
| 86:1:3943:OHX:N3  | 86:1:4200:OHX:N4  | 2.51                     | 0.58              |
| 1:6:138:A:N6      | 1:6:266:A:H61     | 2.01                     | 0.58              |
| 6:s4:11:ARG:N     | 6:s4:26:CYS:O     | 2.31                     | 0.58              |
| 10:s8:5:ARG:HD3   | 10:s8:29:LEU:O    | 2.02                     | 0.58              |
| 36:5:783:A:OP2    | 86:5:4191:OHX:N6  | 2.37                     | 0.58              |
| 36:5:1596:C:H2'   | 36:5:1597:C:C6    | 2.39                     | 0.58              |
| 36:5:1614:C:H2'   | 36:5:1615:C:H6    | 1.68                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:5:3278:C:O2'   | 36:5:3279:A:OP2   | 2.21                     | 0.58              |
| 42:l5:279:LYS:HD3 | 42:l5:282:ARG:CZ  | 2.33                     | 0.58              |
| 52:m6:16:VAL:HG21 | 52:m6:43:ILE:HG12 | 1.83                     | 0.58              |
| 56:n0:12:ARG:HG3  | 56:n0:13:ARG:O    | 2.03                     | 0.58              |
| 86:2:2091:OHX:N5  | 86:2:2132:OHX:N2  | 2.52                     | 0.58              |
| 10:S8:152:ILE:O   | 10:S8:153:GLU:HB2 | 2.03                     | 0.58              |
| 36:1:2105:G:C2'   | 36:1:2106:A:H5'   | 2.33                     | 0.58              |
| 36:1:2873:U:H5''  | 36:1:2873:U:O2    | 2.03                     | 0.58              |
| 42:L5:114:GLY:C   | 42:L5:116:ASP:H   | 2.10                     | 0.58              |
| 53:M7:92:GLN:HA   | 53:M7:95:LEU:HB2  | 1.86                     | 0.58              |
| 55:M9:17:VAL:HG21 | 55:M9:52:LYS:HE3  | 1.84                     | 0.58              |
| 60:N4:6:ASP:HB3   | 60:N4:10:GLY:H    | 1.67                     | 0.58              |
| 67:O1:79:ARG:H    | 67:O1:79:ARG:NE   | 2.00                     | 0.58              |
| 70:O4:20:ILE:HD11 | 70:O4:34:HIS:CE1  | 2.39                     | 0.58              |
| 1:6:1559:A:H5''   | 20:c8:135:GLY:H   | 1.68                     | 0.58              |
| 1:6:1657:U:O2'    | 1:6:1658:G:OP2    | 2.10                     | 0.58              |
| 1:6:1669:U:OP2    | 86:6:2190:OHX:N3  | 2.36                     | 0.58              |
| 10:s8:8:ARG:NH2   | 10:s8:22:ARG:HE   | 2.02                     | 0.58              |
| 33:e1:96:LYS:O    | 33:e1:97:LYS:HB3  | 2.03                     | 0.58              |
| 36:5:1070:U:O4    | 86:5:4110:OHX:N6  | 2.36                     | 0.58              |
| 36:5:2854:U:P     | 47:m0:3:ARG:HH22  | 2.27                     | 0.58              |
| 36:5:3035:A:OP2   | 86:5:4051:OHX:N5  | 2.36                     | 0.58              |
| 86:8:215:OHX:N6   | 86:8:223:OHX:N3   | 2.50                     | 0.58              |
| 41:l4:141:ARG:NH1 | 41:l4:180:LYS:HD3 | 2.18                     | 0.58              |
| 1:2:1459:C:OP2    | 20:C8:138:THR:OG1 | 2.20                     | 0.58              |
| 2:S0:182:LEU:HB3  | 2:S0:188:LEU:HD23 | 1.85                     | 0.58              |
| 19:C7:5:ARG:O     | 19:C7:10:LYS:HE2  | 2.04                     | 0.58              |
| 36:1:353:G:N7     | 73:O7:55:ARG:HD3  | 2.18                     | 0.58              |
| 36:1:1322:U:OP1   | 56:N0:117:ARG:HD2 | 2.04                     | 0.58              |
| 36:1:1581:C:H2'   | 36:1:1582:C:H5''  | 1.86                     | 0.58              |
| 36:1:2828:G:OP1   | 47:M0:7:ARG:NH1   | 2.37                     | 0.58              |
| 1:6:158:U:O2'     | 1:6:159:U:H3'     | 2.03                     | 0.58              |
| 1:6:332:U:P       | 10:s8:56:ARG:HH22 | 2.26                     | 0.58              |
| 1:6:374:U:OP1     | 13:c1:96:LYS:NZ   | 2.30                     | 0.58              |
| 1:6:407:A:H2'     | 1:6:408:C:C6      | 2.39                     | 0.58              |
| 1:6:775:G:N7      | 26:d4:11:LYS:NZ   | 2.51                     | 0.58              |
| 28:d6:10:ARG:HB2  | 28:d6:34:LYS:HA   | 1.86                     | 0.58              |
| 86:8:215:OHX:N6   | 86:8:223:OHX:N4   | 2.52                     | 0.58              |
| 45:l8:54:GLU:O    | 45:l8:58:VAL:HG23 | 2.04                     | 0.58              |
| 65:n9:23:LYS:HB3  | 65:n9:24:PRO:HD3  | 1.86                     | 0.58              |
| 1:2:866:G:OP1     | 15:C3:2:GLY:HA2   | 2.04                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:1291:G:H22    | 1:2:1324:G:N2      | 2.01                     | 0.58              |
| 7:S5:62:VAL:HG13  | 7:S5:89:ILE:HG12   | 1.86                     | 0.58              |
| 8:S6:64:LYS:O     | 8:S6:67:VAL:HG22   | 2.04                     | 0.58              |
| 17:C5:15:HIS:HB3  | 17:C5:22:LEU:HD23  | 1.86                     | 0.58              |
| 36:1:715:A:H8     | 64:N8:115:LYS:HG2  | 1.69                     | 0.58              |
| 36:1:1478:C:H2'   | 36:1:1479:U:H6     | 1.69                     | 0.58              |
| 36:1:1636:U:H5''  | 63:N7:73:LYS:HZ1   | 1.67                     | 0.58              |
| 40:L3:76:VAL:HG12 | 40:L3:325:LYS:HA   | 1.83                     | 0.58              |
| 79:Q3:56:THR:HB   | 79:Q3:63:THR:OG1   | 2.03                     | 0.58              |
| 1:6:1219:A:N3     | 12:c0:51:SER:OG    | 2.35                     | 0.58              |
| 7:s5:203:LYS:HE2  | 7:s5:203:LYS:HA    | 1.84                     | 0.58              |
| 9:s7:49:ILE:HG13  | 9:s7:57:ALA:HB3    | 1.86                     | 0.58              |
| 30:d8:44:VAL:HG11 | 30:d8:48:VAL:HG21  | 1.86                     | 0.58              |
| 36:5:3053:G:OP2   | 86:5:4170:OHX:N3   | 2.37                     | 0.58              |
| 45:l8:113:ALA:O   | 45:l8:115:ALA:N    | 2.34                     | 0.58              |
| 45:l8:116:VAL:C   | 45:l8:118:GLU:H    | 2.11                     | 0.58              |
| 45:l8:161:GLU:HA  | 45:l8:164:VAL:HG22 | 1.85                     | 0.58              |
| 51:m5:184:LYS:H   | 51:m5:186:GLY:H    | 1.52                     | 0.58              |
| 53:m7:109:ALA:HA  | 53:m7:112:LEU:HD22 | 1.85                     | 0.58              |
| 56:n0:96:ASP:OD1  | 56:n0:97:VAL:N     | 2.31                     | 0.58              |
| 1:2:138:A:O2'     | 8:S6:149:LYS:NZ    | 2.37                     | 0.58              |
| 1:2:868:G:OP1     | 15:C3:121:ARG:NH1  | 2.36                     | 0.58              |
| 1:2:919:A:H5'     | 16:C4:18:ARG:HH12  | 1.68                     | 0.58              |
| 1:2:1483:A:H2'    | 1:2:1484:G:C8      | 2.39                     | 0.58              |
| 86:2:2091:OHX:N1  | 86:2:2132:OHX:N4   | 2.52                     | 0.58              |
| 36:1:772:U:H2'    | 36:1:773:G:C8      | 2.39                     | 0.58              |
| 86:1:4007:OHX:N3  | 86:1:4175:OHX:N5   | 2.51                     | 0.58              |
| 40:L3:25:ILE:H    | 40:L3:25:ILE:CD1   | 2.17                     | 0.58              |
| 51:M5:46:ASP:OD1  | 51:M5:50:ARG:NH2   | 2.37                     | 0.58              |
| 68:O2:40:SER:O    | 68:O2:44:ARG:HG3   | 2.03                     | 0.58              |
| 1:6:190:C:N4      | 1:6:196:G:O6       | 2.37                     | 0.58              |
| 15:c3:148:ALA:O   | 86:c3:201:OHX:N4   | 2.37                     | 0.58              |
| 17:c5:60:LEU:HD23 | 17:c5:76:VAL:HG21  | 1.86                     | 0.58              |
| 36:5:2799:A:H1'   | 64:n8:42:ARG:NH2   | 2.19                     | 0.58              |
| 43:l6:3:ALA:HB2   | 68:o2:77:ALA:HB2   | 1.86                     | 0.58              |
| 53:m7:29:THR:HG22 | 53:m7:87:SER:OG    | 2.04                     | 0.58              |
| 56:n0:26:ARG:HH11 | 57:n1:150:THR:HG21 | 1.69                     | 0.58              |
| 70:o4:38:LEU:H    | 70:o4:38:LEU:HD12  | 1.69                     | 0.58              |
| 74:o8:64:LYS:HG3  | 74:o8:65:LEU:N     | 2.19                     | 0.58              |
| 1:2:1097:U:O4     | 4:S2:201:ASN:ND2   | 2.36                     | 0.58              |
| 14:C2:36:LEU:HD21 | 14:C2:102:GLY:HA3  | 1.86                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:768:C:OP1     | 49:M3:186:ARG:NH2  | 2.37                     | 0.58              |
| 36:1:3308:C:N3     | 53:M7:69:ARG:NH1   | 2.51                     | 0.58              |
| 39:L2:13:GLY:O     | 39:L2:17:THR:HG23  | 2.03                     | 0.58              |
| 41:L4:35:VAL:HG21  | 41:L4:244:LEU:HD21 | 1.85                     | 0.58              |
| 42:L5:155:THR:HG22 | 42:L5:179:ARG:HH11 | 1.67                     | 0.58              |
| 62:N6:43:TYR:CD1   | 62:N6:126:LEU:HA   | 2.39                     | 0.58              |
| 1:6:647:G:H1       | 1:6:687:G:H1       | 1.52                     | 0.58              |
| 1:6:1000:C:N4      | 1:6:1003:A:OP2     | 2.37                     | 0.58              |
| 1:6:1680:G:O6      | 86:6:2189:OHX:N1   | 2.37                     | 0.58              |
| 7:s5:35:GLN:C      | 7:s5:37:GLN:H      | 2.11                     | 0.58              |
| 9:s7:168:SER:O     | 9:s7:172:VAL:HG23  | 2.04                     | 0.58              |
| 40:l3:77:THR:CG2   | 40:l3:327:CYS:HA   | 2.34                     | 0.58              |
| 49:m3:16:LYS:O     | 49:m3:17:HIS:HB2   | 2.03                     | 0.58              |
| 59:n3:3:GLY:HA2    | 59:n3:40:LYS:HB3   | 1.86                     | 0.58              |
| 86:2:2037:OHX:N2   | 10:S8:17:LYS:O     | 2.37                     | 0.57              |
| 2:S0:193:GLN:O     | 2:S0:195:TRP:N     | 2.37                     | 0.57              |
| 10:S8:21:PHE:O     | 10:S8:22:ARG:HG2   | 2.04                     | 0.57              |
| 27:D5:44:GLN:NE2   | 27:D5:48:ASP:OD2   | 2.37                     | 0.57              |
| 36:1:1365:G:OP2    | 86:1:3971:OHX:N6   | 2.37                     | 0.57              |
| 37:3:60:G:H2'      | 37:3:61:G:H8       | 1.68                     | 0.57              |
| 1:6:700:C:H2'      | 1:6:701:U:C6       | 2.39                     | 0.57              |
| 15:c3:18:TYR:O     | 15:c3:19:SER:HB2   | 2.05                     | 0.57              |
| 80:e0:14:VAL:O     | 80:e0:18:THR:HG23  | 2.04                     | 0.57              |
| 36:5:996:A:H2'     | 36:5:997:A:O4'     | 2.04                     | 0.57              |
| 36:5:1098:A:OP2    | 57:n1:130:ARG:HD3  | 2.04                     | 0.57              |
| 36:5:1808:G:O6     | 86:5:4024:OHX:N3   | 2.36                     | 0.57              |
| 36:5:1878:G:OP1    | 86:5:3957:OHX:N5   | 2.37                     | 0.57              |
| 36:5:2397:A:OP1    | 36:5:2398:A:H5''   | 2.03                     | 0.57              |
| 36:5:3242:G:H5'    | 36:5:3245:A:H8     | 1.69                     | 0.57              |
| 36:5:3275:U:H4'    | 36:5:3276:G:OP2    | 2.04                     | 0.57              |
| 63:n7:46:ILE:HD11  | 63:n7:49:TYR:CD2   | 2.39                     | 0.57              |
| 3:S1:176:VAL:HG12  | 3:S1:177:GLN:H     | 1.69                     | 0.57              |
| 22:D0:69:LYS:HE2   | 22:D0:80:GLU:HB2   | 1.86                     | 0.57              |
| 36:1:385:A:H2'     | 36:1:386:A:C8      | 2.39                     | 0.57              |
| 36:1:562:C:H2'     | 36:1:563:U:H6      | 1.67                     | 0.57              |
| 86:1:4036:OHX:N6   | 86:1:4048:OHX:N3   | 2.52                     | 0.57              |
| 40:L3:296:THR:HG22 | 40:L3:298:PHE:N    | 2.19                     | 0.57              |
| 43:L6:31:ARG:NH1   | 69:O3:107:ILE:O    | 2.34                     | 0.57              |
| 49:M3:76:THR:HG22  | 49:M3:101:ARG:HB3  | 1.85                     | 0.57              |
| 66:O0:99:ASP:O     | 66:O0:103:THR:HG23 | 2.04                     | 0.57              |
| 1:6:217:A:C8       | 1:6:218:A:C8       | 2.92                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:c7:29:GLN:HG2   | 34:sR:67:ILE:HD11  | 1.85                     | 0.57              |
| 58:n2:43:VAL:HG23  | 58:n2:49:ASN:HB3   | 1.86                     | 0.57              |
| 83:p1:38:UNK:O     | 83:p1:42:UNK:N     | 2.37                     | 0.57              |
| 1:2:312:A:C2       | 1:2:314:C:H2'      | 2.39                     | 0.57              |
| 1:2:542:A:H5''     | 1:2:544:A:C8       | 2.40                     | 0.57              |
| 1:2:780:A:H8       | 26:D4:8:ARG:HB3    | 1.68                     | 0.57              |
| 7:S5:143:ARG:HD3   | 30:D8:55:VAL:HG11  | 1.87                     | 0.57              |
| 13:C1:3:THR:HG1    | 13:C1:82:ARG:HE    | 1.49                     | 0.57              |
| 14:C2:54:ARG:O     | 14:C2:56:GLU:N     | 2.32                     | 0.57              |
| 25:D3:73:ARG:HE    | 25:D3:84:THR:HG22  | 1.69                     | 0.57              |
| 37:3:60:G:H2'      | 37:3:61:G:C8       | 2.38                     | 0.57              |
| 16:c4:61:MET:O     | 16:c4:65:GLN:HG2   | 2.05                     | 0.57              |
| 36:5:917:A:OP2     | 86:5:4222:OHX:N3   | 2.38                     | 0.57              |
| 36:5:920:A:OP1     | 36:5:922:U:H5      | 1.87                     | 0.57              |
| 36:5:1015:U:O3'    | 36:5:1016:C:H2'    | 2.04                     | 0.57              |
| 38:8:154:C:H5''    | 45:l8:181:LYS:HD3  | 1.86                     | 0.57              |
| 42:l5:122:VAL:HG23 | 42:l5:123:GLU:N    | 2.18                     | 0.57              |
| 50:m4:55:ARG:HD3   | 56:n0:70:THR:OG1   | 2.04                     | 0.57              |
| 56:n0:48:LEU:C     | 56:n0:49:HIS:HD1   | 2.13                     | 0.57              |
| 62:n6:115:ARG:HH11 | 62:n6:115:ARG:HG3  | 1.70                     | 0.57              |
| 1:2:326:G:OP1      | 13:C1:57:LYS:NZ    | 2.35                     | 0.57              |
| 1:2:862:A:N7       | 15:C3:64:ARG:NH2   | 2.49                     | 0.57              |
| 1:2:1127:G:OP1     | 77:Q1:11:ARG:NH2   | 2.36                     | 0.57              |
| 1:2:1248:C:H2'     | 1:2:1249:U:H6      | 1.69                     | 0.57              |
| 1:2:1629:G:H2'     | 1:2:1630:U:C6      | 2.40                     | 0.57              |
| 5:S3:127:MET:HE1   | 5:S3:133:GLY:HA2   | 1.86                     | 0.57              |
| 9:S7:131:PHE:HB3   | 9:S7:132:PRO:HD3   | 1.85                     | 0.57              |
| 14:C2:124:LYS:O    | 14:C2:126:TRP:N    | 2.37                     | 0.57              |
| 27:D5:41:ILE:HG13  | 27:D5:42:LEU:HG    | 1.86                     | 0.57              |
| 86:1:3976:OHX:N6   | 86:1:4159:OHX:N4   | 2.52                     | 0.57              |
| 41:L4:120:TYR:CE2  | 41:L4:277:PRO:HB3  | 2.39                     | 0.57              |
| 43:L6:129:GLU:OE2  | 43:L6:130:ILE:N    | 2.37                     | 0.57              |
| 51:M5:85:THR:HG22  | 86:Q2:503:OHX:N1   | 2.19                     | 0.57              |
| 1:6:469:C:H2'      | 1:6:470:A:H5''     | 1.86                     | 0.57              |
| 1:6:767:U:C5       | 11:s9:143:ILE:HD13 | 2.39                     | 0.57              |
| 1:6:1720:G:O6      | 86:6:2094:OHX:N4   | 2.38                     | 0.57              |
| 6:s4:204:GLY:HA2   | 86:s4:301:OHX:N6   | 2.20                     | 0.57              |
| 36:5:1152:G:H22    | 36:5:1200:A:H61    | 1.50                     | 0.57              |
| 36:5:2896:A:H5''   | 36:5:2896:A:H8     | 1.70                     | 0.57              |
| 86:8:215:OHX:N2    | 86:8:223:OHX:N4    | 2.52                     | 0.57              |
| 57:n1:14:MET:HE1   | 57:n1:55:LYS:HB2   | 1.86                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:C6:49:TYR:HB3  | 18:C6:53:LEU:HD21  | 1.86                     | 0.57              |
| 24:D2:104:LEU:HB2 | 24:D2:125:ILE:HA   | 1.87                     | 0.57              |
| 36:1:20:A:OP2     | 71:O5:90:ARG:NH1   | 2.38                     | 0.57              |
| 36:1:2818:U:H6    | 36:1:2818:U:C5'    | 2.17                     | 0.57              |
| 36:1:3160:U:H2'   | 36:1:3161:C:C6     | 2.38                     | 0.57              |
| 86:1:3976:OHX:N3  | 86:1:4159:OHX:N4   | 2.53                     | 0.57              |
| 42:L5:294:ALA:C   | 42:L5:296:GLN:H    | 2.10                     | 0.57              |
| 48:M1:15:GLU:HG2  | 48:M1:16:LYS:HD3   | 1.86                     | 0.57              |
| 72:O6:27:SER:O    | 72:O6:28:TYR:HB2   | 2.03                     | 0.57              |
| 1:6:1762:A:C1'    | 1:6:1783:C:H5'     | 2.35                     | 0.57              |
| 3:s1:41:ARG:HH22  | 3:s1:232:HIS:HA    | 1.70                     | 0.57              |
| 6:s4:95:THR:HG23  | 6:s4:97:GLU:HG2    | 1.85                     | 0.57              |
| 22:d0:22:ILE:HG22 | 22:d0:93:LEU:HB2   | 1.87                     | 0.57              |
| 27:d5:58:ARG:HB3  | 27:d5:103:ARG:HH11 | 1.69                     | 0.57              |
| 36:5:30:G:O5'     | 51:m5:172:ARG:HD2  | 2.04                     | 0.57              |
| 36:5:1916:U:O3'   | 55:m9:85:ARG:NH2   | 2.38                     | 0.57              |
| 45:l8:86:THR:O    | 45:l8:90:THR:OG1   | 2.19                     | 0.57              |
| 48:m1:82:ARG:HB3  | 48:m1:112:LEU:HB2  | 1.86                     | 0.57              |
| 71:o5:34:GLN:HB3  | 71:o5:38:ARG:HH22  | 1.69                     | 0.57              |
| 1:2:380:U:H5      | 11:S9:5:PRO:HA     | 1.69                     | 0.57              |
| 1:2:1220:C:OP1    | 12:C0:48:SER:OG    | 2.21                     | 0.57              |
| 5:S3:64:ARG:O     | 5:S3:67:ASN:N      | 2.36                     | 0.57              |
| 7:S5:89:ILE:HD12  | 7:S5:90:ILE:H      | 1.70                     | 0.57              |
| 11:S9:110:GLN:NE2 | 11:S9:126:ARG:HG2  | 2.19                     | 0.57              |
| 18:C6:22:VAL:HG22 | 18:C6:65:ILE:HG12  | 1.86                     | 0.57              |
| 34:SR:76:ASP:OD1  | 34:SR:76:ASP:N     | 2.26                     | 0.57              |
| 36:1:1819:U:O4    | 86:1:4044:OHX:N6   | 2.37                     | 0.57              |
| 36:1:3092:C:O2'   | 36:1:3094:A:OP2    | 2.19                     | 0.57              |
| 40:L3:332:ARG:HG2 | 40:L3:332:ARG:HH11 | 1.69                     | 0.57              |
| 44:L7:54:GLU:OE2  | 44:L7:186:HIS:NE2  | 2.34                     | 0.57              |
| 47:M0:76:MET:HE3  | 47:M0:148:VAL:HA   | 1.86                     | 0.57              |
| 61:N5:82:LEU:HD12 | 61:N5:126:LEU:HD21 | 1.87                     | 0.57              |
| 63:N7:53:VAL:HG21 | 63:N7:62:VAL:HG13  | 1.87                     | 0.57              |
| 78:Q2:17:CYS:SG   | 78:Q2:76:LYS:HB2   | 2.44                     | 0.57              |
| 78:Q2:25:VAL:HG22 | 78:Q2:72:LEU:HD23  | 1.86                     | 0.57              |
| 1:6:542:A:H8      | 1:6:543:C:H5'      | 1.69                     | 0.57              |
| 1:6:830:U:H2'     | 1:6:831:U:H5'      | 1.86                     | 0.57              |
| 5:s3:167:PHE:CE1  | 5:s3:192:PRO:HB3   | 2.39                     | 0.57              |
| 7:s5:43:PHE:N     | 7:s5:46:TRP:O      | 2.34                     | 0.57              |
| 16:c4:82:LYS:HG3  | 16:c4:118:VAL:HG11 | 1.87                     | 0.57              |
| 36:5:1573:G:C6    | 36:5:1574:C:H1'    | 2.39                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:5:2580:A:O2'    | 86:5:4129:OHX:N1  | 2.36                     | 0.57              |
| 36:5:2988:C:OP1    | 52:m6:68:ARG:NH1  | 2.37                     | 0.57              |
| 36:5:3152:U:O2     | 86:5:4224:OHX:N5  | 2.38                     | 0.57              |
| 46:l9:1:MET:O      | 46:l9:2:LYS:HB2   | 2.03                     | 0.57              |
| 1:2:25:C:O2        | 86:2:2085:OHX:N1  | 2.38                     | 0.57              |
| 1:2:199:G:HO2'     | 1:2:200:A:H8      | 1.53                     | 0.57              |
| 1:2:1410:A:H2'     | 1:2:1411:A:O4'    | 2.05                     | 0.57              |
| 3:S1:144:ARG:HB3   | 3:S1:208:GLN:HB3  | 1.85                     | 0.57              |
| 3:S1:154:SER:O     | 3:S1:154:SER:OG   | 2.23                     | 0.57              |
| 22:D0:55:PRO:HA    | 22:D0:91:ILE:HG12 | 1.87                     | 0.57              |
| 36:1:561:C:H2'     | 36:1:562:C:H6     | 1.68                     | 0.57              |
| 36:1:1159:A:O2'    | 36:1:1160:C:H5''  | 2.05                     | 0.57              |
| 38:4:78:G:H2'      | 38:4:79:A:C8      | 2.39                     | 0.57              |
| 40:L3:232:ARG:NH1  | 40:L3:269:GLN:O   | 2.36                     | 0.57              |
| 61:N5:80:ASN:HD21  | 61:N5:126:LEU:HB2 | 1.69                     | 0.57              |
| 73:O7:88:ALA:O     | 86:O7:103:OHX:N1  | 2.36                     | 0.57              |
| 1:6:218:A:H2'      | 1:6:219:A:H5''    | 1.87                     | 0.57              |
| 1:6:235:G:H2'      | 1:6:236:A:H8      | 1.70                     | 0.57              |
| 1:6:486:G:H22      | 1:6:501:U:H3      | 1.52                     | 0.57              |
| 1:6:542:A:H8       | 1:6:543:C:H2'     | 1.67                     | 0.57              |
| 7:s5:61:TYR:HE2    | 7:s5:164:PRO:HG2  | 1.68                     | 0.57              |
| 7:s5:89:ILE:HD12   | 7:s5:90:ILE:H     | 1.69                     | 0.57              |
| 10:s8:44:HIS:O     | 10:s8:56:ARG:N    | 2.37                     | 0.57              |
| 20:c8:91:ASP:O     | 20:c8:92:ILE:HB   | 2.05                     | 0.57              |
| 36:5:1081:U:O2'    | 36:5:1082:U:O5'   | 2.22                     | 0.57              |
| 36:5:2787:G:OP2    | 86:5:4034:OHX:N6  | 2.37                     | 0.57              |
| 36:5:3241:G:H2'    | 36:5:3245:A:H8    | 1.70                     | 0.57              |
| 36:5:3369:G:C6     | 40:l3:380:MET:HE3 | 2.39                     | 0.57              |
| 1:2:1214:U:OP1     | 1:2:1246:C:H1'    | 2.05                     | 0.57              |
| 20:C8:27:LYS:HG3   | 20:C8:57:ARG:HH21 | 1.69                     | 0.57              |
| 86:1:4036:OHX:N4   | 86:1:4048:OHX:N1  | 2.52                     | 0.57              |
| 1:6:931:C:P        | 28:d6:70:LYS:HE3  | 2.45                     | 0.57              |
| 18:c6:18:ALA:HB2   | 18:c6:69:VAL:HG13 | 1.86                     | 0.57              |
| 36:5:2181:C:OP1    | 39:l2:193:ARG:NH2 | 2.37                     | 0.57              |
| 36:5:2440:G:O2'    | 36:5:2441:A:OP1   | 2.23                     | 0.57              |
| 36:5:2942:C:O2     | 86:5:4108:OHX:N2  | 2.38                     | 0.57              |
| 41:l4:182:LEU:HD11 | 41:l4:223:PRO:HG2 | 1.86                     | 0.57              |
| 59:n3:84:SER:HA    | 59:n3:94:TYR:HB3  | 1.86                     | 0.57              |
| 1:2:520:A:H2'      | 1:2:521:A:C8      | 2.39                     | 0.57              |
| 1:2:905:A:H5''     | 16:C4:52:ARG:HD3  | 1.87                     | 0.57              |
| 1:2:1479:A:P       | 21:C9:57:ARG:HH12 | 2.28                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1646:C:H2'     | 1:2:1647:U:C6      | 2.40                     | 0.57              |
| 86:2:2045:OHX:N1   | 86:2:2099:OHX:N3   | 2.53                     | 0.57              |
| 2:S0:200:ASP:HB2   | 19:C7:85:VAL:HG22  | 1.87                     | 0.57              |
| 9:S7:170:GLN:HA    | 9:S7:181:ILE:HG22  | 1.87                     | 0.57              |
| 27:D5:39:ALA:O     | 27:D5:72:GLY:N     | 2.35                     | 0.57              |
| 36:1:2679:A:O2'    | 48:M1:52:TYR:OH    | 2.22                     | 0.57              |
| 36:1:3152:U:O2'    | 36:1:3153:U:H5'    | 2.04                     | 0.57              |
| 46:L9:188:THR:O    | 46:L9:188:THR:OG1  | 2.22                     | 0.57              |
| 52:M6:171:LYS:O    | 52:M6:175:THR:HG23 | 2.04                     | 0.57              |
| 63:N7:4:PHE:CZ     | 66:O0:35:ARG:HA    | 2.40                     | 0.57              |
| 18:c6:6:SER:HA     | 18:c6:23:LYS:HA    | 1.86                     | 0.57              |
| 36:5:979:U:H1'     | 36:5:980:A:N3      | 2.20                     | 0.57              |
| 36:5:1239:C:H42    | 36:5:1249:G:H1     | 1.51                     | 0.57              |
| 36:5:2683:U:H2'    | 36:5:2684:C:C6     | 2.40                     | 0.57              |
| 41:l4:300:ARG:HH11 | 41:l4:300:ARG:CG   | 2.18                     | 0.57              |
| 56:n0:12:ARG:HB3   | 56:n0:24:LEU:HD23  | 1.86                     | 0.57              |
| 56:n0:13:ARG:HG3   | 56:n0:13:ARG:NH1   | 2.20                     | 0.57              |
| 79:q3:50:GLY:O     | 79:q3:54:ILE:HD13  | 2.03                     | 0.57              |
| 3:S1:61:LEU:O      | 3:S1:62:LYS:NZ     | 2.35                     | 0.57              |
| 9:S7:15:GLU:O      | 9:S7:19:GLN:HG2    | 2.05                     | 0.57              |
| 36:1:750:G:P       | 65:N9:40:ARG:HH21  | 2.27                     | 0.57              |
| 36:1:2403:G:H1'    | 36:1:2404:A:H5''   | 1.87                     | 0.57              |
| 36:1:2444:C:H3'    | 36:1:2445:A:H5''   | 1.87                     | 0.57              |
| 39:L2:20:THR:HA    | 39:L2:23:ARG:HD3   | 1.87                     | 0.57              |
| 42:L5:83:LEU:HB3   | 42:L5:88:ILE:HB    | 1.87                     | 0.57              |
| 59:N3:30:GLY:HA3   | 59:N3:66:LYS:HD2   | 1.86                     | 0.57              |
| 1:6:694:U:H3'      | 1:6:695:U:O2       | 2.05                     | 0.57              |
| 1:6:1620:C:H2'     | 1:6:1621:U:H6      | 1.70                     | 0.57              |
| 3:s1:110:LEU:HD11  | 3:s1:213:ARG:HD2   | 1.86                     | 0.57              |
| 17:c5:108:ARG:HH21 | 20:c8:119:ILE:HD12 | 1.70                     | 0.57              |
| 21:c9:33:TYR:HD1   | 21:c9:34:VAL:H     | 1.53                     | 0.57              |
| 21:c9:112:GLY:O    | 21:c9:125:SER:OG   | 2.19                     | 0.57              |
| 36:5:541:U:H2'     | 36:5:542:G:C8      | 2.40                     | 0.57              |
| 36:5:604:G:N7      | 86:5:4166:OHX:N2   | 2.52                     | 0.57              |
| 36:5:1100:U:OP2    | 44:l7:196:LYS:HE2  | 2.05                     | 0.57              |
| 36:5:1450:G:OP1    | 86:5:4227:OHX:N4   | 2.38                     | 0.57              |
| 36:5:1639:C:H5'    | 70:o4:52:GLN:HG2   | 1.87                     | 0.57              |
| 36:5:1696:A:OP2    | 86:5:4183:OHX:N6   | 2.38                     | 0.57              |
| 36:5:1940:G:H21    | 36:5:3362:A:H8     | 1.53                     | 0.57              |
| 40:l3:56:ILE:HD11  | 40:l3:359:ILE:HG12 | 1.86                     | 0.57              |
| 41:l4:8:VAL:O      | 41:l4:16:THR:HB    | 2.05                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:l8:95:ASN:OD1  | 45:l8:98:ARG:NH1   | 2.38                     | 0.57              |
| 48:m1:92:ARG:HH21 | 48:m1:94:ARG:HD2   | 1.69                     | 0.57              |
| 54:m8:182:LYS:NZ  | 64:n8:55:LYS:O     | 2.37                     | 0.57              |
| 1:2:819:G:O2'     | 1:2:821:U:OP2      | 2.13                     | 0.56              |
| 1:2:1339:C:O2'    | 1:2:1340:U:OP1     | 2.23                     | 0.56              |
| 1:2:1796:C:OP2    | 28:D6:5:ARG:NH1    | 2.38                     | 0.56              |
| 3:S1:119:THR:HB   | 3:S1:143:THR:HG23  | 1.87                     | 0.56              |
| 22:D0:34:LEU:HD23 | 22:D0:112:VAL:HG13 | 1.86                     | 0.56              |
| 33:E1:135:HIS:ND1 | 33:E1:138:ARG:HD2  | 2.20                     | 0.56              |
| 36:1:1016:C:O2    | 36:1:1028:U:N3     | 2.38                     | 0.56              |
| 36:1:3148:U:O4    | 86:1:4113:OHX:N2   | 2.38                     | 0.56              |
| 86:1:4088:OHX:N4  | 55:M9:14:VAL:O     | 2.38                     | 0.56              |
| 45:L8:26:LEU:HD13 | 63:N7:53:VAL:HG11  | 1.85                     | 0.56              |
| 69:O3:60:ARG:HB2  | 69:O3:60:ARG:NH2   | 2.20                     | 0.56              |
| 1:6:443:C:OP2     | 26:d4:105:ARG:HB2  | 2.05                     | 0.56              |
| 1:6:902:G:N1      | 16:c4:51:ASP:OD1   | 2.30                     | 0.56              |
| 1:6:1679:G:O6     | 86:6:2189:OHX:N3   | 2.38                     | 0.56              |
| 86:5:4055:OHX:N5  | 86:5:4197:OHX:N6   | 2.53                     | 0.56              |
| 40:l3:10:ARG:NH1  | 40:l3:11:HIS:O     | 2.38                     | 0.56              |
| 41:l4:144:LYS:HG2 | 41:l4:145:ILE:H    | 1.70                     | 0.56              |
| 74:o8:39:ARG:NH1  | 74:o8:63:LYS:HE2   | 2.20                     | 0.56              |
| 1:2:12:U:H2'      | 1:2:13:C:C6        | 2.39                     | 0.56              |
| 1:2:458:G:OP2     | 26:D4:105:ARG:NH2  | 2.38                     | 0.56              |
| 1:2:778:G:H22     | 26:D4:10:ARG:NH2   | 2.03                     | 0.56              |
| 2:S0:198:MET:SD   | 19:C7:85:VAL:HG11  | 2.45                     | 0.56              |
| 7:S5:91:GLU:HA    | 7:S5:94:THR:HG23   | 1.86                     | 0.56              |
| 14:C2:30:VAL:HB   | 14:C2:132:GLU:HG3  | 1.87                     | 0.56              |
| 36:1:623:U:OP1    | 86:1:4135:OHX:N1   | 2.38                     | 0.56              |
| 45:L8:78:PHE:O    | 45:L8:80:TYR:N     | 2.34                     | 0.56              |
| 1:6:66:U:C5       | 8:s6:173:PRO:HG3   | 2.39                     | 0.56              |
| 1:6:143:G:N7      | 8:s6:177:ARG:NH2   | 2.53                     | 0.56              |
| 1:6:639:U:OP2     | 9:s7:119:THR:HG23  | 2.05                     | 0.56              |
| 6:s4:9:LEU:HD12   | 6:s4:30:ARG:HA     | 1.87                     | 0.56              |
| 30:d8:13:ILE:HB   | 30:d8:29:ARG:HG2   | 1.86                     | 0.56              |
| 30:d8:32:PHE:O    | 30:d8:34:GLU:N     | 2.37                     | 0.56              |
| 36:5:201:A:OP2    | 86:5:3987:OHX:N1   | 2.39                     | 0.56              |
| 36:5:655:C:OP1    | 68:o2:27:ARG:HB3   | 2.06                     | 0.56              |
| 36:5:822:G:H1'    | 39:l2:15:ILE:HD12  | 1.87                     | 0.56              |
| 36:5:1447:G:H3'   | 53:m7:67:ILE:HD11  | 1.87                     | 0.56              |
| 36:5:1810:A:H2'   | 36:5:1811:G:C8     | 2.40                     | 0.56              |
| 36:5:2556:C:O2'   | 63:n7:135:ARG:NH2  | 2.38                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:l2:171:GLY:O    | 79:q3:68:ALA:HB2   | 2.05                     | 0.56              |
| 42:l5:152:ARG:HH11 | 42:l5:152:ARG:HG3  | 1.70                     | 0.56              |
| 42:l5:226:TYR:HE1  | 42:l5:236:LEU:HD11 | 1.70                     | 0.56              |
| 46:l9:166:ARG:NH2  | 46:l9:168:ARG:HH12 | 2.02                     | 0.56              |
| 57:n1:14:MET:HE3   | 57:n1:58:GLN:HB2   | 1.87                     | 0.56              |
| 67:o1:46:THR:HG23  | 67:o1:47:ASP:N     | 2.20                     | 0.56              |
| 1:2:355:G:OP2      | 86:2:2037:OHX:N4   | 2.38                     | 0.56              |
| 1:2:704:C:H3'      | 1:2:704:C:OP2      | 2.05                     | 0.56              |
| 1:2:793:A:H5''     | 1:2:794:U:C5       | 2.40                     | 0.56              |
| 6:S4:222:LEU:O     | 6:S4:224:ASN:N     | 2.38                     | 0.56              |
| 11:S9:148:VAL:HG11 | 11:S9:156:ILE:HD11 | 1.86                     | 0.56              |
| 13:C1:59:PRO:HB3   | 13:C1:66:ILE:HD11  | 1.86                     | 0.56              |
| 15:C3:27:LYS:H     | 15:C3:27:LYS:CE    | 2.18                     | 0.56              |
| 15:C3:127:ARG:HG2  | 15:C3:127:ARG:HH11 | 1.69                     | 0.56              |
| 16:C4:85:ALA:N     | 16:C4:119:THR:HG22 | 2.16                     | 0.56              |
| 36:1:261:U:H2'     | 36:1:262:U:C6      | 2.40                     | 0.56              |
| 36:1:2155:G:O2'    | 39:L2:227:ARG:NH2  | 2.37                     | 0.56              |
| 36:1:2872:A:O2'    | 36:1:2873:U:H5'    | 2.05                     | 0.56              |
| 36:1:2943:G:OP2    | 40:L3:2:SER:HB2    | 2.05                     | 0.56              |
| 36:1:2973:G:N7     | 86:1:4102:OHX:N2   | 2.54                     | 0.56              |
| 36:1:3152:U:O2     | 86:1:4147:OHX:N4   | 2.38                     | 0.56              |
| 36:1:3215:A:O5'    | 50:M4:121:MET:HE1  | 2.04                     | 0.56              |
| 36:1:3289:G:N7     | 86:1:4134:OHX:N4   | 2.54                     | 0.56              |
| 86:1:4007:OHX:N5   | 86:1:4175:OHX:N5   | 2.53                     | 0.56              |
| 51:M5:74:PRO:O     | 51:M5:75:VAL:HG22  | 2.05                     | 0.56              |
| 59:N3:81:GLN:NE2   | 59:N3:83:LYS:O     | 2.39                     | 0.56              |
| 62:N6:37:LYS:HE2   | 62:N6:37:LYS:H     | 1.71                     | 0.56              |
| 75:O9:9:ILE:O      | 75:O9:13:MET:HG3   | 2.05                     | 0.56              |
| 77:Q1:22:ALA:HA    | 77:Q1:25:LYS:HG3   | 1.87                     | 0.56              |
| 78:Q2:43:TYR:CZ    | 78:Q2:47:GLN:NE2   | 2.74                     | 0.56              |
| 1:6:484:C:N4       | 1:6:503:G:H1       | 2.02                     | 0.56              |
| 1:6:1535:U:H4'     | 1:6:1535:U:OP1     | 2.05                     | 0.56              |
| 1:6:1698:G:N2      | 1:6:1699:G:N7      | 2.53                     | 0.56              |
| 1:6:1754:A:H4'     | 1:6:1755:A:O5'     | 2.06                     | 0.56              |
| 8:s6:155:ASP:N     | 8:s6:155:ASP:OD2   | 2.38                     | 0.56              |
| 15:c3:22:ALA:HB1   | 15:c3:23:PRO:HA    | 1.86                     | 0.56              |
| 18:c6:99:GLU:HG2   | 34:sR:57:PRO:HB2   | 1.86                     | 0.56              |
| 25:d3:23:ARG:HB3   | 25:d3:29:TYR:CE1   | 2.40                     | 0.56              |
| 34:sR:80:ALA:HB3   | 34:sR:92:TRP:HB2   | 1.88                     | 0.56              |
| 34:sR:133:VAL:O    | 34:sR:141:LEU:N    | 2.29                     | 0.56              |
| 36:5:182:U:H4'     | 36:5:182:U:OP1     | 2.04                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:5:662:U:H2'    | 36:5:663:C:C6     | 2.40                     | 0.56              |
| 36:5:1599:G:OP1   | 86:o4:203:OHX:N4  | 2.39                     | 0.56              |
| 36:5:1876:U:H6    | 36:5:1876:U:C5'   | 2.19                     | 0.56              |
| 36:5:3164:C:H1'   | 36:5:3165:A:H5'   | 1.86                     | 0.56              |
| 36:5:3343:G:N2    | 36:5:3362:A:H2    | 1.91                     | 0.56              |
| 51:m5:163:GLY:HA2 | 51:m5:168:GLY:HA3 | 1.87                     | 0.56              |
| 1:2:527:A:OP2     | 86:2:2054:OHX:N4  | 2.38                     | 0.56              |
| 6:S4:205:PHE:HB3  | 6:S4:221:ARG:HD2  | 1.88                     | 0.56              |
| 7:S5:42:LEU:HD21  | 7:S5:45:LYS:HD2   | 1.87                     | 0.56              |
| 12:C0:14:TYR:CE1  | 12:C0:18:GLU:HG3  | 2.41                     | 0.56              |
| 36:1:437:G:H2'    | 36:1:438:A:C8     | 2.41                     | 0.56              |
| 36:1:658:G:OP1    | 86:1:4049:OHX:N4  | 2.38                     | 0.56              |
| 36:1:1095:U:N3    | 57:N1:127:GLN:OE1 | 2.35                     | 0.56              |
| 88:1:4216:3H3:H3  | 88:1:4216:3H3:C3  | 2.35                     | 0.56              |
| 45:L8:41:GLN:HG3  | 45:L8:44:ARG:HH12 | 1.71                     | 0.56              |
| 1:6:564:G:O6      | 86:6:2154:OHX:N5  | 2.39                     | 0.56              |
| 2:s0:62:ARG:HG3   | 2:s0:62:ARG:NH1   | 2.12                     | 0.56              |
| 2:s0:148:ASP:OD1  | 2:s0:149:LEU:N    | 2.35                     | 0.56              |
| 6:s4:100:ARG:NH2  | 6:s4:122:LYS:HA   | 2.20                     | 0.56              |
| 16:c4:84:ARG:HG3  | 16:c4:85:ALA:O    | 2.05                     | 0.56              |
| 36:5:22:G:H1'     | 38:8:104:A:N3     | 2.20                     | 0.56              |
| 36:5:412:G:OP1    | 53:m7:62:ARG:NH1  | 2.38                     | 0.56              |
| 36:5:1560:G:O2'   | 36:5:1561:G:OP1   | 2.23                     | 0.56              |
| 36:5:1581:C:OP2   | 36:5:1581:C:H4'   | 2.03                     | 0.56              |
| 36:5:1659:U:H2'   | 36:5:1660:C:C6    | 2.40                     | 0.56              |
| 36:5:3005:A:H5'   | 40:l3:98:GLY:HA3  | 1.88                     | 0.56              |
| 36:5:3279:A:H2'   | 36:5:3280:U:H5'   | 1.88                     | 0.56              |
| 39:l2:68:LYS:HG2  | 39:l2:70:ARG:HG2  | 1.88                     | 0.56              |
| 40:l3:2:SER:O     | 40:l3:3:HIS:HB3   | 2.03                     | 0.56              |
| 40:l3:256:HIS:HA  | 40:l3:257:PRO:C   | 2.31                     | 0.56              |
| 41:l4:148:ILE:HA  | 41:l4:149:PRO:C   | 2.29                     | 0.56              |
| 3:S1:40:ASN:ND2   | 3:S1:42:ASN:O     | 2.39                     | 0.56              |
| 3:S1:119:THR:HB   | 3:S1:143:THR:CG2  | 2.36                     | 0.56              |
| 20:C8:41:ARG:NE   | 21:C9:46:PRO:HD3  | 2.20                     | 0.56              |
| 36:1:1064:A:H4'   | 36:1:1065:A:O5'   | 2.05                     | 0.56              |
| 36:1:2406:C:H2'   | 36:1:2407:C:C6    | 2.40                     | 0.56              |
| 36:1:2510:U:O2'   | 36:1:2511:A:H5''  | 2.05                     | 0.56              |
| 45:L8:195:SER:O   | 45:L8:197:VAL:N   | 2.38                     | 0.56              |
| 66:O0:16:LEU:HB3  | 66:O0:98:SER:HB2  | 1.87                     | 0.56              |
| 70:O4:74:ARG:HG2  | 70:O4:75:ALA:H    | 1.71                     | 0.56              |
| 1:6:336:G:H2'     | 1:6:338:C:H5      | 1.70                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:s2:203:LYS:O     | 4:s2:206:THR:HG23  | 2.06                     | 0.56              |
| 13:c1:132:SER:O    | 13:c1:132:SER:OG   | 2.17                     | 0.56              |
| 17:c5:22:LEU:HA    | 17:c5:25:LEU:HD12  | 1.86                     | 0.56              |
| 36:5:39:A:H5''     | 64:n8:35:ALA:HB2   | 1.88                     | 0.56              |
| 36:5:1258:U:O2     | 36:5:1260:A:H8     | 1.88                     | 0.56              |
| 86:5:4055:OHX:N1   | 86:5:4197:OHX:N2   | 2.54                     | 0.56              |
| 54:m8:166:LEU:O    | 54:m8:167:SER:HB2  | 2.05                     | 0.56              |
| 1:2:1229:G:H1      | 14:C2:47:GLU:HG3   | 1.69                     | 0.56              |
| 36:1:1507:G:C8     | 53:M7:129:THR:HG22 | 2.40                     | 0.56              |
| 36:1:1804:A:H2'    | 36:1:1805:C:C6     | 2.41                     | 0.56              |
| 36:1:2592:G:H4'    | 36:1:2594:C:C2     | 2.39                     | 0.56              |
| 36:1:3318:G:OP2    | 36:1:3318:G:H2'    | 2.05                     | 0.56              |
| 37:3:121:U:OP2     | 42:L5:265:TYR:OH   | 2.15                     | 0.56              |
| 40:L3:2:SER:O      | 40:L3:3:HIS:HB3    | 2.06                     | 0.56              |
| 43:L6:175:LYS:O    | 50:M4:117:ARG:NH2  | 2.39                     | 0.56              |
| 67:O1:13:THR:HG22  | 67:O1:72:ARG:HD3   | 1.87                     | 0.56              |
| 74:O8:42:LYS:HG2   | 74:O8:55:VAL:HG22  | 1.87                     | 0.56              |
| 1:6:140:A:H1'      | 8:s6:179:VAL:HG21  | 1.86                     | 0.56              |
| 1:6:230:C:H42      | 1:6:235:G:H1       | 1.52                     | 0.56              |
| 4:s2:53:ILE:HD11   | 4:s2:73:LEU:HD13   | 1.87                     | 0.56              |
| 5:s3:60:GLY:HA3    | 5:s3:65:ARG:HB3    | 1.88                     | 0.56              |
| 7:s5:37:GLN:OE1    | 18:c6:53:LEU:HD22  | 2.05                     | 0.56              |
| 7:s5:68:ILE:HD13   | 7:s5:69:PHE:H      | 1.70                     | 0.56              |
| 36:5:291:C:OP1     | 51:m5:68:ARG:HG3   | 2.05                     | 0.56              |
| 36:5:2549:G:N3     | 45:l8:33:ASN:ND2   | 2.54                     | 0.56              |
| 36:5:2568:C:O2'    | 36:5:2569:A:O5'    | 2.16                     | 0.56              |
| 36:5:2998:U:O4     | 86:5:4140:OHX:N4   | 2.38                     | 0.56              |
| 36:5:3241:G:H2'    | 36:5:3245:A:C8     | 2.40                     | 0.56              |
| 41:l4:192:GLY:HA2  | 41:l4:195:ARG:HG3  | 1.86                     | 0.56              |
| 44:l7:157:ASN:O    | 44:l7:158:LYS:HB3  | 2.06                     | 0.56              |
| 48:m1:92:ARG:NH2   | 48:m1:94:ARG:HD2   | 2.20                     | 0.56              |
| 52:m6:127:LEU:HD11 | 56:n0:168:PRO:HG3  | 1.88                     | 0.56              |
| 77:q1:9:ARG:HH11   | 77:q1:9:ARG:CG     | 2.17                     | 0.56              |
| 10:S8:26:LYS:O     | 10:S8:26:LYS:HG3   | 2.06                     | 0.56              |
| 22:D0:80:GLU:HG3   | 31:D9:54:LYS:HZ3   | 1.71                     | 0.56              |
| 35:SM:101:ASP:O    | 35:SM:102:THR:HB   | 2.05                     | 0.56              |
| 36:1:1564:U:H2'    | 36:1:1565:G:C8     | 2.40                     | 0.56              |
| 1:6:1178:G:H4'     | 35:sM:83:LYS:HE2   | 1.86                     | 0.56              |
| 1:6:1199:G:O6      | 22:d0:67:THR:HG22  | 2.06                     | 0.56              |
| 86:6:2060:OHX:N2   | 86:6:2147:OHX:N4   | 2.54                     | 0.56              |
| 5:s3:74:GLN:HA     | 5:s3:79:TYR:HB2    | 1.88                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:c5:122:THR:HG22 | 17:c5:123:TYR:HD1  | 1.69                     | 0.56              |
| 29:d7:2:VAL:O      | 29:d7:3:LEU:HB2    | 2.05                     | 0.56              |
| 36:5:129:U:H2'     | 36:5:130:A:C8      | 2.40                     | 0.56              |
| 86:5:4011:OHX:N3   | 86:5:4198:OHX:N5   | 2.53                     | 0.56              |
| 45:l8:24:ASN:HB3   | 45:l8:25:PRO:HD2   | 1.87                     | 0.56              |
| 47:m0:30:LYS:HG3   | 47:m0:63:GLU:OE1   | 2.05                     | 0.56              |
| 4:S2:170:ILE:HB    | 4:S2:197:TYR:HB2   | 1.87                     | 0.56              |
| 6:S4:185:GLY:N     | 6:S4:189:LEU:HD13  | 2.20                     | 0.56              |
| 22:D0:46:GLU:HB2   | 22:D0:52:LYS:NZ    | 2.20                     | 0.56              |
| 36:1:2614:G:OP1    | 86:1:4179:OHX:N6   | 2.39                     | 0.56              |
| 37:3:10:C:OP2      | 57:N1:26:HIS:HD2   | 1.88                     | 0.56              |
| 40:L3:36:ASP:OD1   | 40:L3:38:SER:OG    | 2.20                     | 0.56              |
| 44:L7:150:LYS:HD3  | 44:L7:244:ASN:HD21 | 1.71                     | 0.56              |
| 46:L9:106:LYS:H    | 46:L9:109:ALA:CB   | 2.19                     | 0.56              |
| 1:6:1558:U:H3      | 17:c5:122:THR:HG22 | 1.70                     | 0.56              |
| 1:6:1631:A:OP2     | 86:6:2168:OHX:N3   | 2.38                     | 0.56              |
| 2:s0:168:HIS:O     | 2:s0:172:LEU:HB2   | 2.06                     | 0.56              |
| 17:c5:7:ALA:C      | 17:c5:9:LYS:H      | 2.13                     | 0.56              |
| 86:5:4055:OHX:N3   | 86:5:4197:OHX:N6   | 2.54                     | 0.56              |
| 86:5:4094:OHX:N3   | 86:5:4234:OHX:N4   | 2.54                     | 0.56              |
| 41:l4:316:ASN:O    | 41:l4:319:LYS:O    | 2.24                     | 0.56              |
| 42:l5:254:LYS:HG3  | 42:l5:254:LYS:O    | 2.03                     | 0.56              |
| 48:m1:139:THR:HG22 | 48:m1:146:GLY:O    | 2.05                     | 0.56              |
| 54:m8:67:ILE:HG23  | 54:m8:81:VAL:HG11  | 1.88                     | 0.56              |
| 56:n0:48:LEU:O     | 56:n0:49:HIS:ND1   | 2.36                     | 0.56              |
| 67:o1:10:ARG:HH12  | 67:o1:44:MET:HG3   | 1.70                     | 0.56              |
| 1:2:1798:U:C5      | 28:D6:38:ARG:NH2   | 2.74                     | 0.56              |
| 86:2:2091:OHX:N3   | 86:2:2132:OHX:N4   | 2.53                     | 0.56              |
| 34:SR:81:LEU:HG    | 34:SR:91:LEU:HD13  | 1.87                     | 0.56              |
| 36:1:1874:A:OP2    | 55:M9:21:LYS:HE2   | 2.05                     | 0.56              |
| 36:1:3008:A:OP2    | 52:M6:74:ARG:NH1   | 2.37                     | 0.56              |
| 36:1:3165:A:H2'    | 36:1:3166:C:C6     | 2.41                     | 0.56              |
| 86:1:4032:OHX:N2   | 86:1:4149:OHX:N5   | 2.53                     | 0.56              |
| 12:c0:1:MET:HE3    | 12:c0:2:LEU:H      | 1.71                     | 0.56              |
| 15:c3:53:LEU:HD13  | 29:d7:52:THR:HG21  | 1.87                     | 0.56              |
| 17:c5:127:ARG:CZ   | 35:sM:66:ALA:HB2   | 2.36                     | 0.56              |
| 33:e1:90:LYS:HD3   | 33:e1:93:HIS:HE1   | 1.71                     | 0.56              |
| 33:e1:91:ILE:HG12  | 33:e1:92:LYS:HG2   | 1.88                     | 0.56              |
| 36:5:983:A:OP1     | 65:n9:22:LYS:HA    | 2.06                     | 0.56              |
| 39:l2:70:ARG:CZ    | 39:l2:72:ARG:HE    | 2.18                     | 0.56              |
| 50:m4:47:ASP:CG    | 50:m4:55:ARG:HB2   | 2.31                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:n4:32:GLN:OE1   | 60:n4:33:ASN:ND2   | 2.38                     | 0.56              |
| 1:2:918:U:O3'      | 16:C4:18:ARG:NH1   | 2.39                     | 0.56              |
| 1:2:1041:G:H2'     | 1:2:1042:G:C8      | 2.40                     | 0.56              |
| 1:2:1202:A:H61     | 1:2:1457:C:H5''    | 1.70                     | 0.56              |
| 14:C2:74:LEU:HD11  | 33:E1:106:TYR:HD1  | 1.70                     | 0.56              |
| 18:C6:109:PHE:CD2  | 18:C6:117:LEU:HD21 | 2.41                     | 0.56              |
| 21:C9:118:PRO:HD2  | 21:C9:123:ARG:NH2  | 2.21                     | 0.56              |
| 36:1:619:A:H5''    | 36:1:620:U:OP1     | 2.06                     | 0.56              |
| 36:1:1103:A:H2'    | 36:1:1103:A:N3     | 2.20                     | 0.56              |
| 40:L3:303:LYS:HZ2  | 40:L3:361:THR:HB   | 1.71                     | 0.56              |
| 64:N8:65:GLN:O     | 64:N8:66:ALA:HB2   | 2.06                     | 0.56              |
| 73:O7:21:ARG:NH2   | 73:O7:41:ALA:O     | 2.29                     | 0.56              |
| 1:6:660:G:H2'      | 1:6:661:A:H4'      | 1.88                     | 0.56              |
| 1:6:1588:G:OP1     | 86:6:2125:OHX:N2   | 2.39                     | 0.56              |
| 1:6:1796:C:H5      | 28:d6:6:ALA:H      | 1.52                     | 0.56              |
| 86:6:2060:OHX:N1   | 86:6:2147:OHX:N4   | 2.54                     | 0.56              |
| 2:s0:62:ARG:HH11   | 2:s0:62:ARG:CG     | 2.18                     | 0.56              |
| 7:s5:61:TYR:OH     | 30:d8:52:ASP:OD1   | 2.18                     | 0.56              |
| 7:s5:94:THR:HG22   | 7:s5:114:ILE:CG1   | 2.36                     | 0.56              |
| 7:s5:187:ILE:H     | 7:s5:187:ILE:HD12  | 1.71                     | 0.56              |
| 26:d4:121:THR:HG22 | 26:d4:123:LYS:HB2  | 1.88                     | 0.56              |
| 36:5:110:G:OP2     | 49:m3:73:ARG:NH1   | 2.39                     | 0.56              |
| 36:5:410:U:O4      | 86:5:4102:OHX:N1   | 2.39                     | 0.56              |
| 36:5:914:A:C2      | 39:l2:204:MET:HG2  | 2.41                     | 0.56              |
| 44:l7:158:LYS:HD2  | 44:l7:159:GLN:HA   | 1.88                     | 0.56              |
| 1:2:271:A:H5'      | 1:2:272:U:OP2      | 2.06                     | 0.55              |
| 7:S5:182:ALA:O     | 7:S5:186:ASN:ND2   | 2.39                     | 0.55              |
| 36:1:1119:C:OP2    | 86:1:3958:OHX:N1   | 2.39                     | 0.55              |
| 36:1:2529:A:OP1    | 45:L8:248:LYS:NZ   | 2.39                     | 0.55              |
| 40:L3:66:LYS:HE3   | 59:N3:124:ASP:OD2  | 2.06                     | 0.55              |
| 1:6:169:A:H5''     | 8:s6:176:GLN:HG2   | 1.88                     | 0.55              |
| 8:s6:73:ILE:HD12   | 8:s6:75:LEU:HD21   | 1.87                     | 0.55              |
| 18:c6:115:THR:HG23 | 18:c6:118:ILE:O    | 2.06                     | 0.55              |
| 26:d4:29:HIS:HB2   | 26:d4:67:GLY:HA2   | 1.87                     | 0.55              |
| 54:m8:122:ILE:HD11 | 54:m8:130:ARG:NH1  | 2.20                     | 0.55              |
| 82:p0:25:LEU:HB3   | 82:p0:191:TYR:HB3  | 1.87                     | 0.55              |
| 86:2:2045:OHX:N1   | 86:2:2099:OHX:N5   | 2.54                     | 0.55              |
| 24:D2:89:TRP:O     | 24:D2:93:LEU:HD22  | 2.06                     | 0.55              |
| 41:L4:232:SER:O    | 41:L4:233:LEU:HB2  | 2.05                     | 0.55              |
| 46:L9:120:ASP:OD1  | 46:L9:124:ARG:NH2  | 2.39                     | 0.55              |
| 66:O0:9:SER:OG     | 66:O0:10:ILE:N     | 2.39                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:1091:A:H4'     | 1:6:1092:A:O5'     | 2.07                     | 0.55              |
| 1:6:1699:G:C2      | 1:6:1701:A:H5''    | 2.40                     | 0.55              |
| 1:6:1767:G:OP1     | 1:6:1770:U:H4'     | 2.06                     | 0.55              |
| 8:s6:49:VAL:HB     | 8:s6:115:LYS:HG2   | 1.88                     | 0.55              |
| 37:7:60:G:N2       | 42:l5:274:GLN:OE1  | 2.32                     | 0.55              |
| 42:l5:261:THR:HG23 | 42:l5:264:GLN:HE21 | 1.71                     | 0.55              |
| 71:o5:34:GLN:HB3   | 71:o5:38:ARG:NH2   | 2.20                     | 0.55              |
| 1:2:407:A:H2'      | 1:2:408:C:C6       | 2.42                     | 0.55              |
| 1:2:1783:C:H2'     | 1:2:1784:C:H6      | 1.71                     | 0.55              |
| 10:S8:39:GLY:N     | 10:S8:60:ILE:O     | 2.33                     | 0.55              |
| 18:C6:73:GLY:H     | 18:C6:76:SER:HB2   | 1.71                     | 0.55              |
| 36:1:544:C:H1'     | 36:1:548:G:H22     | 1.71                     | 0.55              |
| 36:1:1949:G:OP1    | 55:M9:104:ARG:NH1  | 2.39                     | 0.55              |
| 36:1:2318:U:O4     | 86:1:4043:OHX:N2   | 2.40                     | 0.55              |
| 36:1:2433:U:H1'    | 51:M5:125:SER:HB3  | 1.88                     | 0.55              |
| 36:1:2854:U:H5''   | 47:M0:160:PRO:HD3  | 1.88                     | 0.55              |
| 36:1:3159:C:H2'    | 36:1:3160:U:H6     | 1.70                     | 0.55              |
| 40:L3:10:ARG:NH1   | 40:L3:11:HIS:O     | 2.39                     | 0.55              |
| 1:6:354:C:H5''     | 10:s8:16:ALA:HB2   | 1.89                     | 0.55              |
| 15:c3:55:ARG:HD2   | 15:c3:56:ASP:OD1   | 2.05                     | 0.55              |
| 67:o1:80:ASN:HA    | 67:o1:90:PHE:CE2   | 2.41                     | 0.55              |
| 1:2:260:U:H3'      | 1:2:261:U:C5'      | 2.37                     | 0.55              |
| 1:2:1449:U:H2'     | 1:2:1450:U:C6      | 2.41                     | 0.55              |
| 4:S2:98:PHE:CE1    | 35:SM:116:GLU:HG3  | 2.42                     | 0.55              |
| 14:C2:73:LYS:NZ    | 33:E1:108:VAL:HG13 | 2.22                     | 0.55              |
| 22:D0:46:GLU:CD    | 22:D0:52:LYS:HE2   | 2.32                     | 0.55              |
| 36:1:742:G:N7      | 86:1:3979:OHX:N1   | 2.54                     | 0.55              |
| 36:1:792:G:H2'     | 36:1:793:C:C6      | 2.42                     | 0.55              |
| 36:1:1581:C:C2     | 36:1:1582:C:H5'    | 2.41                     | 0.55              |
| 36:1:2860:U:H6     | 36:1:2860:U:H5'    | 1.71                     | 0.55              |
| 86:1:4084:OHX:N2   | 86:1:4153:OHX:N1   | 2.54                     | 0.55              |
| 46:L9:147:SER:HB2  | 46:L9:187:ILE:HD11 | 1.88                     | 0.55              |
| 63:N7:46:ILE:HD11  | 63:N7:48:ARG:C     | 2.30                     | 0.55              |
| 68:O2:9:ILE:HG12   | 68:O2:63:THR:HB    | 1.88                     | 0.55              |
| 29:d7:62:ILE:HG13  | 29:d7:63:LEU:H     | 1.70                     | 0.55              |
| 35:sM:58:GLU:O     | 35:sM:62:ARG:HB2   | 2.06                     | 0.55              |
| 36:5:209:A:OP1     | 41:l4:161:LYS:NZ   | 2.39                     | 0.55              |
| 36:5:830:A:O2'     | 36:5:1866:C:H2'    | 2.06                     | 0.55              |
| 86:5:3973:OHX:N4   | 86:5:4241:OHX:N2   | 2.54                     | 0.55              |
| 42:l5:55:PHE:CZ    | 42:l5:158:ARG:HB3  | 2.41                     | 0.55              |
| 46:l9:90:MET:O     | 46:l9:91:ARG:HD2   | 2.06                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 76:q0:77:ILE:O    | 76:q0:78:ILE:HG23 | 2.06                     | 0.55              |
| 78:q2:46:LYS:O    | 86:q2:502:OHX:N3  | 2.39                     | 0.55              |
| 1:2:885:G:H21     | 16:C4:123:SER:HB2 | 1.72                     | 0.55              |
| 1:2:1244:A:O2'    | 1:2:1245:G:OP1    | 2.21                     | 0.55              |
| 23:D1:41:GLU:OE2  | 23:D1:41:GLU:N    | 2.40                     | 0.55              |
| 27:D5:59:TYR:HE2  | 27:D5:61:SER:HB3  | 1.71                     | 0.55              |
| 28:D6:36:ILE:HG21 | 28:D6:78:ALA:HB2  | 1.89                     | 0.55              |
| 36:1:155:G:H5''   | 36:1:156:G:C8     | 2.41                     | 0.55              |
| 36:1:2946:A:H5''  | 36:1:2947:G:H5'   | 1.87                     | 0.55              |
| 36:1:3153:U:O2    | 36:1:3158:G:N1    | 2.39                     | 0.55              |
| 40:L3:188:ILE:HA  | 40:L3:191:LYS:HD2 | 1.89                     | 0.55              |
| 54:M8:86:THR:HG22 | 54:M8:105:ARG:HB2 | 1.88                     | 0.55              |
| 55:M9:130:ASN:C   | 55:M9:132:PHE:H   | 2.13                     | 0.55              |
| 63:N7:10:VAL:HB   | 63:N7:83:THR:HG21 | 1.86                     | 0.55              |
| 63:N7:83:THR:HG23 | 63:N7:85:TYR:N    | 2.21                     | 0.55              |
| 64:N8:74:ASN:HB2  | 64:N8:76:ASP:HB2  | 1.87                     | 0.55              |
| 1:6:404:G:H2'     | 1:6:405:C:C6      | 2.42                     | 0.55              |
| 1:6:656:G:H2'     | 1:6:657:U:C6      | 2.41                     | 0.55              |
| 1:6:1542:G:N2     | 1:6:1568:C:H1'    | 2.22                     | 0.55              |
| 19:c7:109:LEU:O   | 19:c7:113:LEU:HB2 | 2.06                     | 0.55              |
| 36:5:689:U:O4     | 41:14:209:TYR:OH  | 2.16                     | 0.55              |
| 36:5:860:G:O5'    | 39:12:181:LYS:NZ  | 2.39                     | 0.55              |
| 36:5:945:C:H2'    | 36:5:946:U:C6     | 2.42                     | 0.55              |
| 36:5:1149:G:N2    | 36:5:1198:C:N3    | 2.45                     | 0.55              |
| 36:5:2140:U:O2'   | 36:5:2978:U:H5'   | 2.06                     | 0.55              |
| 36:5:2509:U:H2'   | 36:5:2510:U:H5''  | 1.87                     | 0.55              |
| 36:5:3186:A:C2    | 46:19:44:THR:HG22 | 2.42                     | 0.55              |
| 71:o5:6:ALA:O     | 71:o5:10:ARG:HG3  | 2.05                     | 0.55              |
| 1:2:1175:U:H2'    | 1:2:1176:G:C8     | 2.42                     | 0.55              |
| 9:S7:35:LYS:O     | 9:S7:37:GLU:N     | 2.32                     | 0.55              |
| 11:S9:160:PRO:O   | 11:S9:167:ALA:HB2 | 2.06                     | 0.55              |
| 13:C1:53:TYR:CD1  | 13:C1:113:PRO:HG2 | 2.42                     | 0.55              |
| 21:C9:57:ARG:NH2  | 21:C9:80:TYR:HB3  | 2.21                     | 0.55              |
| 36:1:1819:U:O4    | 86:1:4044:OHX:N4  | 2.40                     | 0.55              |
| 36:1:2883:U:H2'   | 36:1:2884:C:C6    | 2.41                     | 0.55              |
| 69:O3:90:PRO:O    | 69:O3:91:ALA:HB3  | 2.06                     | 0.55              |
| 71:O5:119:LYS:HE2 | 71:O5:119:LYS:HA  | 1.88                     | 0.55              |
| 1:6:901:G:N2      | 16:c4:54:GLU:OE1  | 2.40                     | 0.55              |
| 33:e1:144:CYS:O   | 33:e1:146:SER:N   | 2.40                     | 0.55              |
| 36:5:136:G:H5'    | 71:o5:95:PHE:CD2  | 2.41                     | 0.55              |
| 36:5:2549:G:N2    | 45:l8:33:ASN:HA   | 2.22                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:l6:89:THR:HG21 | 50:m4:115:PHE:HB2 | 1.87                     | 0.55              |
| 70:o4:81:CYS:HG   | 70:o4:84:CYS:HG   | 1.52                     | 0.55              |
| 72:o6:43:LEU:HD13 | 72:o6:47:ILE:HD11 | 1.88                     | 0.55              |
| 1:2:61:A:H8       | 1:2:269:G:O2'     | 1.89                     | 0.55              |
| 1:2:867:G:H5'     | 15:C3:4:MET:HE3   | 1.87                     | 0.55              |
| 1:2:1145:U:O2'    | 4:S2:89:GLN:O     | 2.19                     | 0.55              |
| 1:2:1735:U:OP2    | 59:N3:32:ARG:NH1  | 2.40                     | 0.55              |
| 2:S0:177:LEU:O    | 2:S0:181:VAL:HG13 | 2.07                     | 0.55              |
| 9:S7:150:GLN:HB3  | 9:S7:181:ILE:HD12 | 1.88                     | 0.55              |
| 18:C6:58:ASP:C    | 18:C6:60:PHE:H    | 2.15                     | 0.55              |
| 20:C8:95:GLY:O    | 86:C8:201:OHX:N2  | 2.40                     | 0.55              |
| 21:C9:28:LEU:CD1  | 21:C9:29:GLU:H    | 2.20                     | 0.55              |
| 26:D4:60:PHE:H    | 26:D4:71:GLY:HA2  | 1.72                     | 0.55              |
| 36:1:171:G:H2'    | 36:1:172:G:O4'    | 2.06                     | 0.55              |
| 36:1:624:G:OP2    | 86:1:4135:OHX:N3  | 2.39                     | 0.55              |
| 36:1:1171:G:O6    | 86:1:3962:OHX:N2  | 2.40                     | 0.55              |
| 36:1:1413:G:N7    | 86:1:4125:OHX:N4  | 2.55                     | 0.55              |
| 36:1:3195:U:O2'   | 36:1:3197:G:N2    | 2.40                     | 0.55              |
| 36:1:3259:U:H5'   | 36:1:3259:U:C6    | 2.42                     | 0.55              |
| 37:3:85:G:O6      | 86:3:216:OHX:N4   | 2.40                     | 0.55              |
| 44:L7:120:THR:HB  | 57:N1:132:PRO:HB2 | 1.88                     | 0.55              |
| 46:L9:180:TYR:HB2 | 76:Q0:85:LEU:HD13 | 1.89                     | 0.55              |
| 1:6:9:U:O4        | 86:6:2146:OHX:N3  | 2.39                     | 0.55              |
| 2:s0:185:ARG:HB2  | 23:d1:45:ALA:HB3  | 1.89                     | 0.55              |
| 18:c6:7:VAL:HG12  | 18:c6:22:VAL:HB   | 1.89                     | 0.55              |
| 20:c8:33:THR:HA   | 20:c8:38:VAL:HG23 | 1.89                     | 0.55              |
| 36:5:1824:U:OP1   | 74:o8:3:ARG:NH2   | 2.40                     | 0.55              |
| 37:7:3:U:H2'      | 37:7:4:U:C6       | 2.42                     | 0.55              |
| 40:l3:339:ARG:HG2 | 40:l3:340:LYS:O   | 2.07                     | 0.55              |
| 43:l6:175:LYS:O   | 43:l6:176:PHE:HB2 | 2.06                     | 0.55              |
| 44:l7:151:ARG:HD2 | 44:l7:244:ASN:OD1 | 2.07                     | 0.55              |
| 1:2:191:C:O2'     | 1:2:192:U:O5'     | 2.25                     | 0.55              |
| 1:2:1370:U:H1'    | 1:2:1371:A:OP2    | 2.07                     | 0.55              |
| 1:2:1518:C:OP1    | 86:2:2121:OHX:N5  | 2.40                     | 0.55              |
| 1:2:1535:U:O2'    | 1:2:1536:G:N3     | 2.38                     | 0.55              |
| 5:S3:144:ALA:HB1  | 35:SM:101:ASP:OD2 | 2.07                     | 0.55              |
| 6:S4:151:ASP:HB3  | 6:S4:154:ILE:HG13 | 1.89                     | 0.55              |
| 7:S5:37:GLN:OE1   | 18:C6:53:LEU:HD22 | 2.07                     | 0.55              |
| 26:D4:23:PHE:HE2  | 26:D4:75:VAL:HG12 | 1.71                     | 0.55              |
| 36:1:1717:U:H2'   | 36:1:1718:G:C8    | 2.42                     | 0.55              |
| 36:1:2310:U:OP1   | 86:1:4142:OHX:N4  | 2.40                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:2664:C:OP2    | 48:M1:142:LYS:NZ   | 2.39                     | 0.55              |
| 36:1:2718:U:OP1    | 78:Q2:13:LYS:NZ    | 2.40                     | 0.55              |
| 36:1:2927:C:H2'    | 36:1:2928:C:C6     | 2.41                     | 0.55              |
| 36:1:3246:G:O6     | 86:1:4111:OHX:N4   | 2.39                     | 0.55              |
| 36:1:3393:U:H2'    | 36:1:3394:U:H6     | 1.72                     | 0.55              |
| 38:4:69:U:OP2      | 86:O7:103:OHX:N3   | 2.40                     | 0.55              |
| 45:L8:134:TYR:CG   | 45:L8:190:VAL:HG21 | 2.42                     | 0.55              |
| 63:N7:88:ASP:HB3   | 63:N7:121:ARG:NH2  | 2.20                     | 0.55              |
| 1:6:7:G:N7         | 4:s2:205:ARG:NH2   | 2.54                     | 0.55              |
| 1:6:25:C:O2        | 86:6:2108:OHX:N6   | 2.40                     | 0.55              |
| 1:6:1490:C:H4'     | 1:6:1491:U:OP1     | 2.05                     | 0.55              |
| 1:6:1796:C:C2      | 28:d6:5:ARG:HG2    | 2.42                     | 0.55              |
| 86:6:2060:OHX:N1   | 86:6:2147:OHX:N3   | 2.54                     | 0.55              |
| 3:s1:157:GLN:OE1   | 86:s1:302:OHX:N3   | 2.39                     | 0.55              |
| 7:s5:119:ASP:O     | 7:s5:123:VAL:HG23  | 2.07                     | 0.55              |
| 8:s6:98:ARG:HD2    | 8:s6:99:GLY:N      | 2.22                     | 0.55              |
| 30:d8:11:LYS:HB2   | 30:d8:33:LEU:HD23  | 1.88                     | 0.55              |
| 40:l3:361:THR:HG22 | 40:l3:371:GLN:HB3  | 1.89                     | 0.55              |
| 41:l4:38:VAL:HG21  | 41:l4:121:ALA:HB2  | 1.88                     | 0.55              |
| 53:m7:31:GLU:HG3   | 53:m7:60:PHE:HA    | 1.89                     | 0.55              |
| 1:2:226:A:H2'      | 1:2:227:U:H5'      | 1.89                     | 0.55              |
| 1:2:1550:A:OP2     | 17:C5:42:ARG:NH2   | 2.40                     | 0.55              |
| 21:C9:28:LEU:HD13  | 21:C9:29:GLU:H     | 1.71                     | 0.55              |
| 36:1:1744:G:O6     | 86:1:4098:OHX:N2   | 2.40                     | 0.55              |
| 36:1:1919:G:N7     | 86:1:4017:OHX:N5   | 2.55                     | 0.55              |
| 36:1:3159:C:H2'    | 36:1:3160:U:C6     | 2.42                     | 0.55              |
| 50:M4:108:ARG:NH2  | 52:M6:196:ALA:O    | 2.39                     | 0.55              |
| 79:Q3:73:THR:HG22  | 79:Q3:75:ALA:N     | 2.20                     | 0.55              |
| 1:6:1166:A:H2'     | 1:6:1167:G:O4'     | 2.07                     | 0.55              |
| 1:6:1639:C:OP1     | 86:6:2156:OHX:N5   | 2.40                     | 0.55              |
| 34:sR:63:GLY:HA3   | 34:sR:90:ARG:NH1   | 2.22                     | 0.55              |
| 36:5:1556:C:C5     | 36:5:2169:G:C4     | 2.95                     | 0.55              |
| 36:5:1657:C:N4     | 36:5:1798:A:OP2    | 2.36                     | 0.55              |
| 36:5:1724:U:H1'    | 36:5:1725:C:C6     | 2.42                     | 0.55              |
| 36:5:1766:G:H8     | 55:m9:46:LYS:HZ1   | 1.52                     | 0.55              |
| 86:5:4094:OHX:N5   | 86:5:4234:OHX:N6   | 2.55                     | 0.55              |
| 49:m3:75:PHE:H     | 49:m3:97:VAL:HA    | 1.72                     | 0.55              |
| 70:o4:81:CYS:O     | 70:o4:83:ASN:N     | 2.40                     | 0.55              |
| 1:2:1217:A:H8      | 1:2:1217:A:H5'     | 1.72                     | 0.55              |
| 6:S4:104:ASP:HB3   | 6:S4:106:LYS:H     | 1.72                     | 0.55              |
| 22:D0:118:VAL:HG22 | 22:D0:119:ALA:H    | 1.72                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:D4:132:ARG:C    | 26:D4:134:ALA:H    | 2.15                     | 0.55              |
| 36:1:565:U:H2'     | 36:1:566:G:H8      | 1.72                     | 0.55              |
| 36:1:2947:G:C2     | 40:L3:250:ALA:HB1  | 2.41                     | 0.55              |
| 86:1:4036:OHX:N4   | 86:1:4048:OHX:N3   | 2.54                     | 0.55              |
| 45:L8:74:THR:HB    | 45:L8:230:LYS:HZ1  | 1.72                     | 0.55              |
| 46:L9:86:TYR:CE2   | 46:L9:151:VAL:HG22 | 2.42                     | 0.55              |
| 53:M7:28:ASN:O     | 53:M7:32:THR:HG22  | 2.07                     | 0.55              |
| 53:M7:60:PHE:CE2   | 53:M7:82:ARG:HB2   | 2.42                     | 0.55              |
| 55:M9:23:TRP:CH2   | 55:M9:25:ASP:HB2   | 2.43                     | 0.55              |
| 1:6:66:U:H5        | 8:s6:173:PRO:HG3   | 1.73                     | 0.55              |
| 1:6:1213:G:O6      | 86:6:2073:OHX:N6   | 2.40                     | 0.55              |
| 4:s2:176:SER:HB2   | 4:s2:195:ASP:HB3   | 1.89                     | 0.55              |
| 17:c5:43:ARG:NH1   | 17:c5:47:ARG:HD3   | 2.21                     | 0.55              |
| 26:d4:44:LEU:HA    | 26:d4:47:VAL:HG13  | 1.89                     | 0.55              |
| 33:e1:90:LYS:HD3   | 33:e1:93:HIS:CE1   | 2.42                     | 0.55              |
| 36:5:1192:C:N4     | 36:5:1301:A:O3'    | 2.39                     | 0.55              |
| 36:5:1655:G:H8     | 36:5:1655:G:C5'    | 2.20                     | 0.55              |
| 36:5:2397:A:H8     | 36:5:2941:A:N1     | 2.05                     | 0.55              |
| 36:5:3227:A:H2'    | 36:5:3228:C:H5'    | 1.88                     | 0.55              |
| 48:m1:28:ASP:HA    | 48:m1:31:THR:HG23  | 1.89                     | 0.55              |
| 49:m3:93:ILE:HG22  | 49:m3:94:GLY:H     | 1.72                     | 0.55              |
| 51:m5:96:ARG:HG2   | 51:m5:96:ARG:HH11  | 1.72                     | 0.55              |
| 63:n7:29:HIS:HB2   | 63:n7:40:HIS:O     | 2.07                     | 0.55              |
| 1:2:1620:C:OP2     | 86:2:2167:OHX:N6   | 2.40                     | 0.54              |
| 16:C4:84:ARG:HB2   | 16:C4:118:VAL:HG23 | 1.89                     | 0.54              |
| 36:1:1831:U:O2'    | 38:4:114:G:OP1     | 2.21                     | 0.54              |
| 36:1:3395:G:N2     | 36:1:3396:U:O4     | 2.33                     | 0.54              |
| 40:L3:103:THR:HG21 | 40:L3:147:GLU:OE2  | 2.07                     | 0.54              |
| 49:M3:24:VAL:HG23  | 49:M3:24:VAL:O     | 2.07                     | 0.54              |
| 69:O3:16:TYR:OH    | 69:O3:91:ALA:HB2   | 2.07                     | 0.54              |
| 1:6:196:G:O2'      | 1:6:197:A:OP2      | 2.25                     | 0.54              |
| 1:6:1263:G:H2'     | 1:6:1264:G:O4'     | 2.07                     | 0.54              |
| 1:6:1350:U:H2'     | 1:6:1351:G:C8      | 2.41                     | 0.54              |
| 9:s7:164:TYR:CE1   | 9:s7:165:LYS:HG3   | 2.42                     | 0.54              |
| 12:c0:15:LEU:HD22  | 12:c0:68:LEU:HD22  | 1.87                     | 0.54              |
| 22:d0:103:ILE:HA   | 22:d0:106:ILE:HG22 | 1.88                     | 0.54              |
| 36:5:528:U:H2'     | 36:5:529:A:H8      | 1.72                     | 0.54              |
| 36:5:1661:G:H2'    | 36:5:1662:G:C8     | 2.42                     | 0.54              |
| 36:5:2364:G:H22    | 36:5:2396:G:H1'    | 1.71                     | 0.54              |
| 36:5:3242:G:H5'    | 36:5:3245:A:C8     | 2.41                     | 0.54              |
| 86:5:4011:OHX:N6   | 86:5:4198:OHX:N2   | 2.54                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:l3:283:TYR:HB3 | 40:l3:323:MET:HE2  | 1.87                     | 0.54              |
| 50:m4:21:VAL:HB   | 50:m4:63:VAL:HG13  | 1.88                     | 0.54              |
| 63:n7:77:TYR:HA   | 63:n7:80:LEU:HD12  | 1.89                     | 0.54              |
| 66:o0:75:ASN:HA   | 66:o0:86:ARG:HB2   | 1.89                     | 0.54              |
| 1:2:1555:A:P      | 17:C5:47:ARG:HH21  | 2.30                     | 0.54              |
| 3:S1:77:GLU:O     | 3:S1:79:HIS:N      | 2.37                     | 0.54              |
| 7:S5:158:GLN:HG2  | 30:D8:66:LEU:HD21  | 1.90                     | 0.54              |
| 14:C2:33:ARG:HA   | 14:C2:36:LEU:HD12  | 1.88                     | 0.54              |
| 14:C2:119:SER:OG  | 14:C2:120:VAL:N    | 2.40                     | 0.54              |
| 20:C8:11:PHE:CD2  | 20:C8:59:GLY:HA3   | 2.42                     | 0.54              |
| 36:1:1221:A:H3'   | 36:1:1222:G:H5''   | 1.87                     | 0.54              |
| 36:1:1240:A:H3'   | 36:1:1241:U:H5'    | 1.90                     | 0.54              |
| 40:L3:53:MET:HG2  | 40:L3:77:THR:HG22  | 1.87                     | 0.54              |
| 46:L9:105:GLU:HG3 | 46:L9:109:ALA:H    | 1.73                     | 0.54              |
| 3:s1:87:ARG:NH2   | 3:s1:89:ASP:OD1    | 2.41                     | 0.54              |
| 6:s4:185:GLY:HA2  | 6:s4:189:LEU:HD22  | 1.89                     | 0.54              |
| 7:s5:161:ASP:OD2  | 30:d8:42:ARG:NH1   | 2.41                     | 0.54              |
| 11:s9:88:GLU:O    | 11:s9:91:LYS:HD2   | 2.08                     | 0.54              |
| 26:d4:49:LYS:HD3  | 26:d4:49:LYS:N     | 2.22                     | 0.54              |
| 36:5:268:A:C4     | 51:m5:12:ARG:HG3   | 2.42                     | 0.54              |
| 36:5:437:G:H1     | 36:5:622:A:H61     | 1.55                     | 0.54              |
| 36:5:438:A:H2'    | 36:5:494:G:N2      | 2.23                     | 0.54              |
| 36:5:2971:A:H5''  | 36:5:2972:G:O5'    | 2.07                     | 0.54              |
| 36:5:3242:G:N7    | 40:l3:150:ARG:HD2  | 2.22                     | 0.54              |
| 37:7:22:A:H1'     | 42:l5:272:TYR:CZ   | 2.42                     | 0.54              |
| 86:8:215:OHX:N5   | 86:8:223:OHX:N3    | 2.54                     | 0.54              |
| 43:l6:176:PHE:H   | 50:m4:117:ARG:NH2  | 2.05                     | 0.54              |
| 57:n1:122:GLN:O   | 57:n1:124:VAL:HG23 | 2.06                     | 0.54              |
| 1:2:789:A:O2'     | 6:S4:106:LYS:NZ    | 2.39                     | 0.54              |
| 1:2:959:U:C6      | 15:C3:17:PRO:HG2   | 2.43                     | 0.54              |
| 22:D0:23:ARG:HB3  | 22:D0:117:VAL:HG12 | 1.88                     | 0.54              |
| 24:D2:30:SER:HB2  | 24:D2:61:ILE:HG13  | 1.89                     | 0.54              |
| 36:1:1229:G:H1    | 36:1:1280:C:H42    | 1.56                     | 0.54              |
| 47:M0:210:ILE:HA  | 47:M0:217:PHE:CE2  | 2.42                     | 0.54              |
| 53:M7:36:ILE:HD11 | 53:M7:95:LEU:HD11  | 1.89                     | 0.54              |
| 62:N6:51:ARG:HB3  | 62:N6:115:ARG:NH2  | 2.20                     | 0.54              |
| 1:6:828:U:H2'     | 1:6:829:A:H5''     | 1.89                     | 0.54              |
| 1:6:1244:A:N3     | 1:6:1244:A:H3'     | 2.23                     | 0.54              |
| 1:6:1703:C:H2'    | 1:6:1704:U:H6      | 1.72                     | 0.54              |
| 86:6:2060:OHX:N5  | 86:6:2147:OHX:N6   | 2.56                     | 0.54              |
| 2:s0:84:ARG:HD3   | 2:s0:203:PHE:O     | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:s4:130:GLN:HB3   | 6:s4:138:TYR:CZ   | 2.42                     | 0.54              |
| 11:s9:3:ARG:HG2    | 11:s9:3:ARG:NH2   | 2.21                     | 0.54              |
| 12:c0:21:VAL:HG12  | 12:c0:66:TYR:HB2  | 1.88                     | 0.54              |
| 14:c2:42:ALA:HB2   | 14:c2:124:LYS:HD2 | 1.89                     | 0.54              |
| 25:d3:103:LEU:HD12 | 25:d3:126:LYS:HD3 | 1.88                     | 0.54              |
| 36:5:308:A:H5'     | 36:5:2223:A:O2'   | 2.06                     | 0.54              |
| 36:5:725:G:H3'     | 36:5:726:G:H5''   | 1.89                     | 0.54              |
| 47:m0:43:VAL:HG21  | 47:m0:197:VAL:HB  | 1.89                     | 0.54              |
| 1:2:753:A:H5'      | 6:S4:221:ARG:HG3  | 1.89                     | 0.54              |
| 1:2:894:U:H2'      | 1:2:895:G:C8      | 2.43                     | 0.54              |
| 1:2:1034:C:OP1     | 15:C3:9:LYS:NZ    | 2.38                     | 0.54              |
| 1:2:1235:C:O2      | 33:E1:138:ARG:NH2 | 2.41                     | 0.54              |
| 1:2:1796:C:H4'     | 1:2:1797:A:OP2    | 2.07                     | 0.54              |
| 3:S1:131:ASP:HB3   | 3:S1:180:THR:CG2  | 2.38                     | 0.54              |
| 3:S1:185:THR:O     | 3:S1:189:ILE:HG13 | 2.07                     | 0.54              |
| 15:C3:36:GLN:OE1   | 15:C3:58:HIS:NE2  | 2.40                     | 0.54              |
| 16:C4:19:ILE:HB    | 16:C4:83:ILE:HD12 | 1.89                     | 0.54              |
| 36:1:1310:G:O6     | 86:1:4031:OHX:N1  | 2.40                     | 0.54              |
| 36:1:2402:A:C5     | 36:1:2871:G:C2    | 2.96                     | 0.54              |
| 86:1:4032:OHX:N6   | 86:1:4149:OHX:N5  | 2.55                     | 0.54              |
| 86:1:4056:OHX:N6   | 86:1:4163:OHX:N4  | 2.56                     | 0.54              |
| 74:O8:26:LYS:NZ    | 74:O8:28:ASN:OD1  | 2.30                     | 0.54              |
| 75:O9:20:ASN:O     | 75:O9:20:ASN:ND2  | 2.41                     | 0.54              |
| 1:6:914:G:H8       | 1:6:914:G:OP2     | 1.90                     | 0.54              |
| 3:s1:71:ALA:HB3    | 16:c4:114:ARG:NH1 | 2.22                     | 0.54              |
| 29:d7:54:VAL:O     | 29:d7:63:LEU:HB2  | 2.08                     | 0.54              |
| 36:5:1480:G:H4'    | 36:5:1481:A:OP1   | 2.07                     | 0.54              |
| 36:5:2507:C:O2'    | 36:5:2508:U:OP1   | 2.24                     | 0.54              |
| 36:5:3047:U:C2'    | 36:5:3048:A:H5'   | 2.37                     | 0.54              |
| 86:5:3978:OHX:N2   | 86:5:4196:OHX:N5  | 2.56                     | 0.54              |
| 86:5:3978:OHX:N4   | 86:5:4196:OHX:N1  | 2.55                     | 0.54              |
| 42:l5:211:LEU:HB3  | 42:l5:219:PHE:HB2 | 1.88                     | 0.54              |
| 61:n5:48:SER:OG    | 61:n5:49:LYS:N    | 2.41                     | 0.54              |
| 62:n6:37:LYS:H     | 62:n6:37:LYS:CD   | 2.19                     | 0.54              |
| 62:n6:82:VAL:O     | 62:n6:84:LYS:N    | 2.41                     | 0.54              |
| 1:2:72:A:C2        | 1:2:73:U:N3       | 2.75                     | 0.54              |
| 1:2:462:G:N7       | 86:2:2144:OHX:N1  | 2.54                     | 0.54              |
| 1:2:487:G:H3'      | 1:2:488:G:H5''    | 1.88                     | 0.54              |
| 86:1:4059:OHX:N6   | 86:1:4166:OHX:N5  | 2.55                     | 0.54              |
| 1:6:1:U:H5''       | 1:6:2:A:OP1       | 2.08                     | 0.54              |
| 1:6:235:G:H2'      | 1:6:236:A:C8      | 2.43                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:6:831:U:O2'      | 1:6:832:U:H5'     | 2.07                     | 0.54              |
| 10:s8:147:ALA:C    | 10:s8:149:SER:H   | 2.16                     | 0.54              |
| 40:l3:227:GLU:HG3  | 40:l3:270:ARG:HE  | 1.71                     | 0.54              |
| 41:l4:179:LEU:HD22 | 41:l4:183:LYS:HG2 | 1.89                     | 0.54              |
| 42:l5:110:LEU:HA   | 42:l5:113:LEU:HB2 | 1.89                     | 0.54              |
| 45:l8:101:THR:OG1  | 45:l8:104:GLU:HG3 | 2.07                     | 0.54              |
| 46:l9:93:VAL:O     | 46:l9:177:ASP:HA  | 2.06                     | 0.54              |
| 1:2:296:U:H2'      | 1:2:297:U:C6      | 2.41                     | 0.54              |
| 1:2:701:U:H3       | 1:2:737:A:N6      | 2.01                     | 0.54              |
| 34:SR:16:HIS:CE1   | 34:SR:43:ILE:HG12 | 2.42                     | 0.54              |
| 36:1:439:C:H3'     | 36:1:440:A:H8     | 1.73                     | 0.54              |
| 36:1:692:A:OP1     | 51:M5:201:ARG:NH2 | 2.40                     | 0.54              |
| 36:1:1024:G:N7     | 86:1:4168:OHX:N6  | 2.55                     | 0.54              |
| 36:1:2726:C:O2'    | 36:1:2727:A:H2'   | 2.08                     | 0.54              |
| 36:1:3033:A:H2'    | 36:1:3034:C:C6    | 2.43                     | 0.54              |
| 36:1:3064:U:O4     | 86:1:4138:OHX:N6  | 2.41                     | 0.54              |
| 36:1:3087:A:P      | 86:1:4184:OHX:N5  | 2.80                     | 0.54              |
| 41:L4:64:SER:HA    | 41:L4:75:PRO:HA   | 1.89                     | 0.54              |
| 51:M5:38:ARG:HG3   | 51:M5:38:ARG:NH1  | 2.23                     | 0.54              |
| 55:M9:17:VAL:CG2   | 55:M9:52:LYS:HE3  | 2.37                     | 0.54              |
| 78:Q2:17:CYS:HB2   | 87:Q2:501:ZN:ZN   | 1.26                     | 0.54              |
| 79:Q3:91:GLU:N     | 79:Q3:91:GLU:OE2  | 2.39                     | 0.54              |
| 1:6:363:G:OP1      | 86:6:2112:OHX:N1  | 2.39                     | 0.54              |
| 1:6:1017:U:H2'     | 1:6:1018:U:C6     | 2.43                     | 0.54              |
| 8:s6:67:VAL:O      | 8:s6:68:LEU:HB2   | 2.06                     | 0.54              |
| 10:s8:36:THR:HB    | 10:s8:57:ALA:O    | 2.07                     | 0.54              |
| 36:5:289:A:C2      | 51:m5:93:LYS:HG3  | 2.42                     | 0.54              |
| 36:5:1412:G:OP1    | 68:o2:105:ARG:NH2 | 2.40                     | 0.54              |
| 36:5:2659:G:H4'    | 36:5:2751:G:O2'   | 2.07                     | 0.54              |
| 86:5:4207:OHX:N1   | 75:o9:48:LYS:O    | 2.40                     | 0.54              |
| 41:l4:139:GLY:O    | 41:l4:141:ARG:NH1 | 2.41                     | 0.54              |
| 46:l9:77:ASN:HA    | 46:l9:80:THR:HG23 | 1.90                     | 0.54              |
| 1:2:14:C:OP2       | 4:S2:206:THR:HG21 | 2.08                     | 0.54              |
| 11:S9:85:VAL:HG12  | 11:S9:99:LEU:HD11 | 1.89                     | 0.54              |
| 34:SR:93:ASP:HB3   | 34:SR:96:THR:HG22 | 1.89                     | 0.54              |
| 36:1:1064:A:H5''   | 36:1:1066:G:O4'   | 2.07                     | 0.54              |
| 36:1:1103:A:H4'    | 36:1:1103:A:OP2   | 2.08                     | 0.54              |
| 38:4:103:G:O6      | 86:4:223:OHX:N4   | 2.40                     | 0.54              |
| 40:L3:188:ILE:HD12 | 40:L3:189:SER:H   | 1.73                     | 0.54              |
| 45:L8:74:THR:HB    | 45:L8:230:LYS:NZ  | 2.22                     | 0.54              |
| 49:M3:128:ARG:NH2  | 71:O5:109:ILE:O   | 2.31                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:M4:21:VAL:HB    | 50:M4:63:VAL:HG13  | 1.88                     | 0.54              |
| 59:N3:66:LYS:HB3   | 59:N3:68:GLU:OE1   | 2.06                     | 0.54              |
| 1:6:485:A:N6       | 1:6:486:G:N3       | 2.55                     | 0.54              |
| 1:6:913:G:H3'      | 1:6:914:G:H5'      | 1.88                     | 0.54              |
| 7:s5:53:VAL:O      | 7:s5:55:ASP:N      | 2.34                     | 0.54              |
| 8:s6:163:THR:HA    | 8:s6:168:THR:HG22  | 1.89                     | 0.54              |
| 15:c3:55:ARG:HD3   | 29:d7:47:PHE:CD1   | 2.43                     | 0.54              |
| 24:d2:37:PHE:CE2   | 24:d2:103:ILE:HD12 | 2.42                     | 0.54              |
| 25:d3:97:ASP:O     | 25:d3:100:ASP:HB2  | 2.07                     | 0.54              |
| 36:5:2211:U:OP2    | 86:5:4221:OHX:N1   | 2.41                     | 0.54              |
| 36:5:2228:A:H5''   | 36:5:2228:A:H8     | 1.72                     | 0.54              |
| 36:5:2765:C:H2'    | 36:5:2766:U:H6     | 1.71                     | 0.54              |
| 36:5:3358:U:H2'    | 36:5:3359:A:C8     | 2.43                     | 0.54              |
| 86:5:4055:OHX:N5   | 86:5:4197:OHX:N2   | 2.55                     | 0.54              |
| 86:5:4094:OHX:N5   | 86:5:4234:OHX:N2   | 2.55                     | 0.54              |
| 37:7:44:C:OP2      | 48:m1:137:ARG:NH2  | 2.40                     | 0.54              |
| 52:m6:58:LEU:HA    | 52:m6:72:HIS:CD2   | 2.43                     | 0.54              |
| 56:n0:81:TYR:HE1   | 56:n0:90:MET:HE3   | 1.73                     | 0.54              |
| 75:o9:44:TRP:CZ3   | 75:o9:45:ARG:HG3   | 2.41                     | 0.54              |
| 1:2:1765:A:OP2     | 86:2:2093:OHX:N5   | 2.41                     | 0.54              |
| 1:2:1786:G:OP1     | 16:C4:136:ARG:NH2  | 2.33                     | 0.54              |
| 15:C3:33:VAL:HG11  | 15:C3:66:ILE:HG12  | 1.88                     | 0.54              |
| 36:1:3295:A:OP2    | 40:L3:126:LYS:N    | 2.29                     | 0.54              |
| 36:1:3340:G:O6     | 86:1:4056:OHX:N4   | 2.41                     | 0.54              |
| 40:L3:111:SER:OG   | 40:L3:113:GLU:HB2  | 2.08                     | 0.54              |
| 41:L4:52:VAL:HG11  | 41:L4:99:MET:HE3   | 1.90                     | 0.54              |
| 41:L4:181:VAL:O    | 41:L4:182:LEU:CB   | 2.56                     | 0.54              |
| 4:s2:116:LYS:HG2   | 4:s2:127:ALA:HB3   | 1.88                     | 0.54              |
| 11:s9:110:GLN:NE2  | 11:s9:126:ARG:HG2  | 2.23                     | 0.54              |
| 35:sM:23:LYS:HE3   | 35:sM:24:GLU:H     | 1.73                     | 0.54              |
| 36:5:420:G:OP2     | 36:5:420:G:O5'     | 2.26                     | 0.54              |
| 36:5:2897:A:H2'    | 36:5:2899:C:C5'    | 2.38                     | 0.54              |
| 37:7:121:U:H5'     | 42:l5:260:PHE:CE2  | 2.43                     | 0.54              |
| 41:l4:299:ILE:HG23 | 54:m8:39:ARG:HB3   | 1.90                     | 0.54              |
| 45:l8:100:GLU:OE2  | 45:l8:108:ARG:NH1  | 2.40                     | 0.54              |
| 68:o2:11:LYS:O     | 68:o2:12:LYS:HB2   | 2.06                     | 0.54              |
| 1:2:158:U:O2'      | 1:2:159:U:H3'      | 2.08                     | 0.54              |
| 1:2:404:G:H2'      | 1:2:405:C:C6       | 2.42                     | 0.54              |
| 1:2:958:U:OP2      | 29:D7:20:LYS:HE3   | 2.08                     | 0.54              |
| 2:S0:187:ALA:O     | 2:S0:188:LEU:HD22  | 2.08                     | 0.54              |
| 9:S7:126:LEU:HD11  | 9:S7:181:ILE:HG12  | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:C6:123:ARG:HG3  | 18:C6:124:PRO:HD2  | 1.89                     | 0.54              |
| 28:D6:17:HIS:CE1   | 28:D6:18:VAL:O     | 2.61                     | 0.54              |
| 34:SR:93:ASP:HB2   | 34:SR:100:TYR:CE1  | 2.42                     | 0.54              |
| 36:1:1422:G:H21    | 43:L6:5:LYS:HZ1    | 1.56                     | 0.54              |
| 38:4:38:U:C4       | 71:O5:89:ARG:HD2   | 2.43                     | 0.54              |
| 41:L4:8:VAL:O      | 41:L4:16:THR:HB    | 2.08                     | 0.54              |
| 42:L5:217:GLU:HG2  | 42:L5:218:ARG:N    | 2.21                     | 0.54              |
| 52:M6:67:THR:HG23  | 86:M6:202:OHX:N4   | 2.23                     | 0.54              |
| 58:N2:36:TYR:OH    | 58:N2:82:LYS:HG2   | 2.08                     | 0.54              |
| 59:N3:68:GLU:CD    | 59:N3:68:GLU:H     | 2.15                     | 0.54              |
| 1:6:152:U:O2       | 1:6:163:G:N2       | 2.41                     | 0.54              |
| 1:6:565:C:N3       | 86:6:2159:OHX:N4   | 2.56                     | 0.54              |
| 1:6:751:G:H2'      | 1:6:752:A:C8       | 2.43                     | 0.54              |
| 1:6:1787:C:OP2     | 16:c4:132:ARG:HB3  | 2.07                     | 0.54              |
| 11:s9:171:ARG:HE   | 11:s9:174:ARG:HB2  | 1.73                     | 0.54              |
| 11:s9:171:ARG:HH11 | 11:s9:174:ARG:HB3  | 1.72                     | 0.54              |
| 14:c2:97:LEU:HD11  | 14:c2:121:VAL:HG22 | 1.90                     | 0.54              |
| 36:5:3:U:H3        | 38:8:156:U:H3      | 1.54                     | 0.54              |
| 36:5:3112:G:O2'    | 46:l9:70:THR:HB    | 2.08                     | 0.54              |
| 36:5:3259:U:C6     | 36:5:3259:U:H5'    | 2.43                     | 0.54              |
| 43:l6:109:GLU:CD   | 43:l6:109:GLU:H    | 2.16                     | 0.54              |
| 56:n0:171:PHE:O    | 56:n0:172:TYR:C    | 2.50                     | 0.54              |
| 1:2:1015:U:OP1     | 86:2:2046:OHX:N3   | 2.41                     | 0.54              |
| 12:C0:1:MET:HG2    | 12:C0:2:LEU:H      | 1.73                     | 0.54              |
| 22:D0:58:LEU:HD12  | 22:D0:88:LYS:HB3   | 1.89                     | 0.54              |
| 22:D0:106:ILE:HG13 | 22:D0:107:THR:H    | 1.73                     | 0.54              |
| 36:1:561:C:H2'     | 36:1:562:C:C6      | 2.43                     | 0.54              |
| 36:1:1495:U:C5     | 36:1:1835:A:N1     | 2.74                     | 0.54              |
| 36:1:1899:G:N7     | 86:1:3935:OHX:N3   | 2.56                     | 0.54              |
| 36:1:2895:G:C2'    | 36:1:2896:A:H5''   | 2.36                     | 0.54              |
| 38:4:52:A:OP1      | 75:O9:21:ARG:NH2   | 2.28                     | 0.54              |
| 40:L3:324:VAL:HG11 | 40:L3:328:ILE:HD13 | 1.90                     | 0.54              |
| 45:L8:90:THR:HA    | 45:L8:214:LEU:HD21 | 1.90                     | 0.54              |
| 53:M7:122:ALA:HB3  | 53:M7:143:PRO:HB2  | 1.89                     | 0.54              |
| 1:6:241:U:H2'      | 1:6:242:U:C6       | 2.43                     | 0.54              |
| 1:6:393:C:H2'      | 1:6:394:C:C6       | 2.43                     | 0.54              |
| 2:s0:28:ASN:OD1    | 2:s0:28:ASN:N      | 2.40                     | 0.54              |
| 4:s2:67:GLN:HA     | 4:s2:70:ASP:HB2    | 1.89                     | 0.54              |
| 6:s4:161:LYS:HB3   | 6:s4:170:THR:O     | 2.08                     | 0.54              |
| 7:s5:93:LEU:HD23   | 7:s5:172:ILE:HG23  | 1.88                     | 0.54              |
| 21:c9:53:TRP:HH2   | 21:c9:100:ILE:HD12 | 1.73                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:7:C:H5''      | 45:l8:193:LYS:HB3  | 1.88                     | 0.54              |
| 36:5:644:G:H2'     | 36:5:2372:A:N7     | 2.22                     | 0.54              |
| 36:5:2317:A:OP2    | 86:5:4185:OHX:N6   | 2.40                     | 0.54              |
| 36:5:2771:U:H2'    | 36:5:2772:C:C6     | 2.43                     | 0.54              |
| 36:5:2962:U:OP1    | 86:5:3978:OHX:N4   | 2.41                     | 0.54              |
| 41:l4:295:ILE:HG23 | 41:l4:299:ILE:HD11 | 1.90                     | 0.54              |
| 59:n3:87:ARG:HH22  | 59:n3:137:VAL:HG22 | 1.72                     | 0.54              |
| 1:2:1158:C:OP2     | 86:2:2174:OHX:N5   | 2.41                     | 0.53              |
| 1:2:1629:G:H2'     | 1:2:1630:U:H6      | 1.74                     | 0.53              |
| 13:C1:3:THR:OG1    | 13:C1:82:ARG:NE    | 2.35                     | 0.53              |
| 26:D4:21:LYS:HB2   | 26:D4:75:VAL:HG13  | 1.90                     | 0.53              |
| 36:1:655:C:H2'     | 36:1:656:A:C8      | 2.43                     | 0.53              |
| 36:1:980:A:C8      | 36:1:980:A:OP2     | 2.57                     | 0.53              |
| 36:1:3089:C:OP1    | 40:L3:222:LYS:NZ   | 2.39                     | 0.53              |
| 38:4:77:A:OP2      | 86:4:224:OHX:N2    | 2.41                     | 0.53              |
| 41:L4:156:LEU:HD23 | 41:L4:159:ILE:HD12 | 1.90                     | 0.53              |
| 1:6:74:U:H5''      | 1:6:75:U:OP2       | 2.07                     | 0.53              |
| 1:6:542:A:H1'      | 1:6:543:C:H5'      | 1.90                     | 0.53              |
| 1:6:737:A:H2'      | 1:6:738:G:C8       | 2.43                     | 0.53              |
| 1:6:1458:G:H5''    | 1:6:1459:C:OP2     | 2.07                     | 0.53              |
| 1:6:1553:G:N7      | 17:c5:43:ARG:NH1   | 2.56                     | 0.53              |
| 1:6:1795:U:O2      | 28:d6:10:ARG:NE    | 2.33                     | 0.53              |
| 2:s0:195:TRP:NE1   | 2:s0:197:ILE:HD13  | 2.24                     | 0.53              |
| 3:s1:175:GLU:HG2   | 3:s1:193:ILE:HD13  | 1.89                     | 0.53              |
| 36:5:1307:G:H5''   | 52:m6:60:LYS:NZ    | 2.23                     | 0.53              |
| 36:5:2204:C:H4'    | 36:5:2205:U:OP1    | 2.08                     | 0.53              |
| 39:l2:48:ILE:HG12  | 79:q3:63:THR:HG22  | 1.91                     | 0.53              |
| 40:l3:345:ASN:OD1  | 40:l3:346:THR:N    | 2.39                     | 0.53              |
| 46:l9:75:VAL:HA    | 46:l9:78:MET:CE    | 2.38                     | 0.53              |
| 65:n9:14:ARG:NH2   | 65:n9:18:ARG:HH11  | 2.06                     | 0.53              |
| 1:2:385:A:OP1      | 10:S8:25:ARG:NH1   | 2.38                     | 0.53              |
| 1:2:702:G:HO2'     | 1:2:703:G:H8       | 1.57                     | 0.53              |
| 1:2:1253:U:H4'     | 33:E1:143:LYS:N    | 2.23                     | 0.53              |
| 1:2:1450:U:H2'     | 1:2:1451:C:C6      | 2.44                     | 0.53              |
| 10:S8:8:ARG:C      | 10:S8:9:HIS:O      | 2.49                     | 0.53              |
| 12:C0:32:HIS:HD2   | 12:C0:35:ILE:HB    | 1.72                     | 0.53              |
| 36:1:3:U:H2'       | 36:1:4:U:O4'       | 2.08                     | 0.53              |
| 36:1:955:U:H2'     | 36:1:956:U:C6      | 2.44                     | 0.53              |
| 36:1:1313:G:OP1    | 52:M6:82:LYS:HE2   | 2.08                     | 0.53              |
| 36:1:2157:G:O6     | 39:L2:152:SER:HB3  | 2.08                     | 0.53              |
| 86:1:4032:OHX:N6   | 86:1:4149:OHX:N3   | 2.55                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:L3:105:VAL:HG21 | 40:L3:148:LEU:HD13 | 1.89                     | 0.53              |
| 40:L3:123:TYR:CZ   | 40:L3:124:LYS:HG3  | 2.44                     | 0.53              |
| 41:L4:136:LEU:HD23 | 41:L4:142:VAL:HG23 | 1.90                     | 0.53              |
| 41:L4:139:GLY:O    | 41:L4:140:HIS:HB2  | 2.07                     | 0.53              |
| 42:L5:57:ASN:C     | 42:L5:58:LYS:HG2   | 2.34                     | 0.53              |
| 42:L5:86:TYR:CE1   | 42:L5:247:ILE:HA   | 2.43                     | 0.53              |
| 46:L9:3:TYR:HA     | 56:N0:142:GLN:OE1  | 2.08                     | 0.53              |
| 46:L9:86:TYR:CD1   | 46:L9:151:VAL:HG13 | 2.42                     | 0.53              |
| 46:L9:90:MET:HE3   | 46:L9:181:VAL:HG23 | 1.90                     | 0.53              |
| 48:M1:162:TRP:CZ2  | 48:M1:166:LYS:HD2  | 2.44                     | 0.53              |
| 56:N0:12:ARG:HB3   | 56:N0:24:LEU:HD23  | 1.90                     | 0.53              |
| 1:6:486:G:N2       | 1:6:487:G:N7       | 2.56                     | 0.53              |
| 1:6:539:G:H8       | 1:6:539:G:OP2      | 1.92                     | 0.53              |
| 5:s3:60:GLY:O      | 5:s3:62:ASN:N      | 2.40                     | 0.53              |
| 23:d1:36:VAL:HG11  | 23:d1:78:LEU:HD21  | 1.89                     | 0.53              |
| 24:d2:7:LEU:HD13   | 24:d2:74:VAL:HG23  | 1.90                     | 0.53              |
| 35:sM:48:ARG:HA    | 36:5:1019:G:OP1    | 2.08                     | 0.53              |
| 36:5:374:A:N3      | 36:5:376:G:H5''    | 2.23                     | 0.53              |
| 36:5:2734:A:OP1    | 86:5:4046:OHX:N6   | 2.41                     | 0.53              |
| 36:5:3074:G:OP1    | 86:5:4118:OHX:N4   | 2.41                     | 0.53              |
| 41:l4:354:VAL:HG11 | 57:n1:143:THR:HG21 | 1.88                     | 0.53              |
| 45:l8:153:ILE:HD13 | 45:l8:166:LEU:HB3  | 1.90                     | 0.53              |
| 48:m1:155:THR:OG1  | 48:m1:158:ASP:HB2  | 2.07                     | 0.53              |
| 53:m7:108:ASP:N    | 53:m7:152:GLU:OE2  | 2.23                     | 0.53              |
| 55:m9:90:PRO:HG2   | 55:m9:93:VAL:HG23  | 1.90                     | 0.53              |
| 63:n7:22:LYS:HE2   | 63:n7:129:TRP:CZ2  | 2.43                     | 0.53              |
| 79:q3:73:THR:HG22  | 79:q3:75:ALA:N     | 2.24                     | 0.53              |
| 1:2:287:G:O2'      | 1:2:288:A:OP2      | 2.25                     | 0.53              |
| 1:2:393:C:H2'      | 1:2:394:C:C6       | 2.44                     | 0.53              |
| 1:2:513:U:OP1      | 11:S9:133:HIS:NE2  | 2.37                     | 0.53              |
| 1:2:523:G:H5'      | 26:D4:60:PHE:O     | 2.09                     | 0.53              |
| 1:2:1191:U:O2'     | 18:C6:142:TYR:O    | 2.18                     | 0.53              |
| 8:S6:153:VAL:O     | 8:S6:155:ASP:N     | 2.41                     | 0.53              |
| 11:S9:104:PHE:O    | 11:S9:147:MET:HE1  | 2.08                     | 0.53              |
| 14:C2:27:ALA:O     | 14:C2:31:VAL:HG23  | 2.08                     | 0.53              |
| 34:SR:267:PRO:HG2  | 34:SR:269:TYR:HE1  | 1.72                     | 0.53              |
| 36:1:719:U:H6      | 36:1:719:U:H5''    | 1.72                     | 0.53              |
| 36:1:785:G:OP1     | 54:M8:66:ARG:NH1   | 2.40                     | 0.53              |
| 36:1:829:U:H3      | 36:1:895:A:H62     | 1.55                     | 0.53              |
| 36:1:1363:A:OP2    | 86:1:4048:OHX:N6   | 2.42                     | 0.53              |
| 45:L8:50:VAL:HG22  | 45:L8:52:TRP:CE2   | 2.43                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:M5:155:VAL:HG23 | 51:M5:156:HIS:ND1  | 2.24                     | 0.53              |
| 1:6:1192:C:O3'     | 18:c6:140:LYS:NZ   | 2.35                     | 0.53              |
| 1:6:1331:A:OP1     | 19:c7:45:ARG:NH2   | 2.42                     | 0.53              |
| 36:5:3243:A:H4'    | 40:l3:95:THR:HG22  | 1.90                     | 0.53              |
| 86:5:3973:OHX:N3   | 86:5:4241:OHX:N2   | 2.57                     | 0.53              |
| 53:m7:87:SER:O     | 53:m7:91:VAL:HG23  | 2.08                     | 0.53              |
| 69:o3:49:ILE:HG23  | 69:o3:100:ILE:HG13 | 1.89                     | 0.53              |
| 76:q0:99:CYS:HB2   | 76:q0:114:LYS:HD3  | 1.91                     | 0.53              |
| 1:2:558:U:O2'      | 1:2:559:C:O5'      | 2.25                     | 0.53              |
| 6:S4:199:GLU:OE1   | 6:S4:201:HIS:HE1   | 1.91                     | 0.53              |
| 12:C0:53:GLY:O     | 12:C0:55:VAL:N     | 2.40                     | 0.53              |
| 36:1:685:G:P       | 49:M3:35:ARG:NH1   | 2.81                     | 0.53              |
| 36:1:871:U:H2'     | 36:1:872:U:C6      | 2.43                     | 0.53              |
| 86:1:4032:OHX:N2   | 86:1:4149:OHX:N1   | 2.56                     | 0.53              |
| 38:4:104:A:C8      | 38:4:105:A:C8      | 2.97                     | 0.53              |
| 38:4:125:U:O2      | 38:4:125:U:H2'     | 2.08                     | 0.53              |
| 40:L3:68:HIS:CD2   | 40:L3:69:LYS:HG3   | 2.43                     | 0.53              |
| 45:L8:94:PHE:HB3   | 45:L8:189:LEU:HD13 | 1.90                     | 0.53              |
| 45:L8:144:GLU:OE1  | 72:O6:36:ARG:NH2   | 2.41                     | 0.53              |
| 48:M1:95:ASN:N     | 48:M1:95:ASN:HD22  | 2.06                     | 0.53              |
| 1:6:956:C:OP2      | 15:c3:12:SER:HB3   | 2.08                     | 0.53              |
| 1:6:1364:G:N2      | 21:c9:3:GLY:HA3    | 2.23                     | 0.53              |
| 3:s1:48:VAL:HG21   | 3:s1:61:LEU:HD22   | 1.89                     | 0.53              |
| 7:s5:35:GLN:O      | 7:s5:37:GLN:N      | 2.42                     | 0.53              |
| 12:c0:50:THR:HG22  | 12:c0:55:VAL:HG22  | 1.89                     | 0.53              |
| 17:c5:111:MET:HG2  | 20:c8:119:ILE:CG1  | 2.38                     | 0.53              |
| 18:c6:114:ARG:O    | 18:c6:115:THR:HB   | 2.08                     | 0.53              |
| 36:5:93:C:OP2      | 36:5:2764:C:O2'    | 2.22                     | 0.53              |
| 36:5:322:U:H5''    | 36:5:323:A:OP1     | 2.09                     | 0.53              |
| 36:5:1024:G:N2     | 36:5:1026:A:OP2    | 2.41                     | 0.53              |
| 36:5:2403:G:N2     | 36:5:2404:A:H62    | 2.05                     | 0.53              |
| 36:5:3049:A:H5'    | 36:5:3049:A:C8     | 2.42                     | 0.53              |
| 36:5:3155:U:OP1    | 86:5:4224:OHX:N2   | 2.41                     | 0.53              |
| 49:m3:79:GLU:OE2   | 49:m3:101:ARG:NH2  | 2.41                     | 0.53              |
| 63:n7:46:ILE:HD11  | 63:n7:49:TYR:CG    | 2.44                     | 0.53              |
| 67:o1:13:THR:HG22  | 67:o1:72:ARG:HD3   | 1.91                     | 0.53              |
| 74:o8:5:ILE:HD12   | 74:o8:52:TYR:HB3   | 1.91                     | 0.53              |
| 78:q2:10:THR:HA    | 78:q2:20:HIS:CD2   | 2.43                     | 0.53              |
| 79:q3:49:ARG:HB2   | 79:q3:55:TRP:CZ3   | 2.44                     | 0.53              |
| 82:p0:48:ARG:HD2   | 82:p0:90:ASN:HB2   | 1.89                     | 0.53              |
| 1:2:229:U:H2'      | 1:2:230:C:C6       | 2.43                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:393:C:H4'      | 1:2:1673:G:O2'     | 2.07                     | 0.53              |
| 1:2:1472:C:OP1     | 7:S5:102:ARG:NH2   | 2.34                     | 0.53              |
| 1:2:1776:A:H2'     | 1:2:1777:G:C8      | 2.43                     | 0.53              |
| 86:2:2045:OHX:N4   | 86:2:2099:OHX:N3   | 2.56                     | 0.53              |
| 11:S9:168:ARG:HD3  | 11:S9:171:ARG:HH11 | 1.74                     | 0.53              |
| 18:C6:143:ARG:HH22 | 35:SM:84:LYS:HZ1   | 1.57                     | 0.53              |
| 36:1:1408:G:P      | 68:O2:33:ARG:HH22  | 2.31                     | 0.53              |
| 36:1:1778:G:O2'    | 36:1:1780:G:OP2    | 2.21                     | 0.53              |
| 38:4:85:G:C8       | 38:4:85:G:H3'      | 2.44                     | 0.53              |
| 46:L9:77:ASN:HB3   | 46:L9:151:VAL:HG21 | 1.89                     | 0.53              |
| 47:M0:38:LYS:HG2   | 47:M0:41:ALA:HB2   | 1.90                     | 0.53              |
| 1:6:788:A:H2'      | 6:s4:19:LEU:HD22   | 1.90                     | 0.53              |
| 1:6:1097:U:O3'     | 4:s2:159:THR:HG21  | 2.08                     | 0.53              |
| 8:s6:105:ASP:OD2   | 8:s6:105:ASP:N     | 2.30                     | 0.53              |
| 9:s7:98:ILE:HG12   | 9:s7:121:VAL:HG21  | 1.90                     | 0.53              |
| 24:d2:18:GLU:OE1   | 24:d2:69:LEU:HB3   | 2.09                     | 0.53              |
| 36:5:956:U:OP1     | 86:5:4152:OHX:N2   | 2.42                     | 0.53              |
| 36:5:996:A:C2      | 36:5:1054:A:C4     | 2.96                     | 0.53              |
| 41:l4:22:LEU:HD11  | 41:l4:26:PHE:HB2   | 1.91                     | 0.53              |
| 45:l8:200:LEU:HD11 | 45:l8:211:LEU:HD21 | 1.91                     | 0.53              |
| 63:n7:104:PRO:O    | 63:n7:108:GLU:HG3  | 2.09                     | 0.53              |
| 2:S0:4:PRO:HB2     | 2:S0:7:PHE:HB2     | 1.89                     | 0.53              |
| 2:S0:52:LYS:HB3    | 23:D1:82:VAL:HG22  | 1.91                     | 0.53              |
| 20:C8:28:ILE:O     | 20:C8:32:LEU:HG    | 2.09                     | 0.53              |
| 24:D2:17:ALA:HB2   | 24:D2:25:VAL:HG13  | 1.89                     | 0.53              |
| 36:1:1577:G:H2'    | 36:1:1578:C:O4'    | 2.08                     | 0.53              |
| 36:1:2505:U:H2'    | 36:1:2506:U:H6     | 1.73                     | 0.53              |
| 36:1:2883:U:H2'    | 36:1:2884:C:H6     | 1.72                     | 0.53              |
| 86:1:4023:OHX:N4   | 86:1:4061:OHX:N2   | 2.56                     | 0.53              |
| 42:L5:34:LYS:HE3   | 57:N1:30:TYR:CZ    | 2.43                     | 0.53              |
| 47:M0:77:THR:HG22  | 47:M0:85:PHE:CZ    | 2.44                     | 0.53              |
| 47:M0:86:HIS:HB3   | 47:M0:139:ARG:HG2  | 1.89                     | 0.53              |
| 51:M5:68:ARG:HG2   | 51:M5:68:ARG:NH1   | 2.20                     | 0.53              |
| 68:O2:50:ILE:HG13  | 68:O2:50:ILE:O     | 2.09                     | 0.53              |
| 1:6:624:G:H2'      | 1:6:625:C:C6       | 2.43                     | 0.53              |
| 1:6:759:U:OP1      | 86:s9:201:OHX:N2   | 2.42                     | 0.53              |
| 1:6:991:G:OP2      | 86:6:2171:OHX:N2   | 2.42                     | 0.53              |
| 2:s0:169:SER:O     | 2:s0:173:ILE:HG12  | 2.09                     | 0.53              |
| 3:s1:131:ASP:CG    | 3:s1:180:THR:HB    | 2.33                     | 0.53              |
| 5:s3:37:VAL:HG12   | 5:s3:50:ILE:HA     | 1.91                     | 0.53              |
| 6:s4:66:MET:HE1    | 6:s4:78:THR:HG23   | 1.90                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:s4:105:VAL:HG11  | 6:s4:245:LYS:H     | 1.73                     | 0.53              |
| 36:5:530:G:O6      | 86:5:3949:OHX:N3   | 2.42                     | 0.53              |
| 36:5:882:A:H2'     | 36:5:883:A:H5''    | 1.91                     | 0.53              |
| 86:5:4001:OHX:N6   | 86:5:4090:OHX:N2   | 2.57                     | 0.53              |
| 86:5:4201:OHX:N6   | 86:8:224:OHX:N5    | 2.56                     | 0.53              |
| 37:7:28:C:H5''     | 48:m1:137:ARG:HG2  | 1.91                     | 0.53              |
| 40:l3:296:THR:HG21 | 40:l3:357:LYS:O    | 2.08                     | 0.53              |
| 41:l4:99:MET:HE3   | 41:l4:102:PRO:CA   | 2.32                     | 0.53              |
| 51:m5:106:VAL:HG11 | 51:m5:132:VAL:HG21 | 1.91                     | 0.53              |
| 70:o4:99:LYS:O     | 70:o4:103:LYS:HG2  | 2.08                     | 0.53              |
| 78:q2:71:ARG:HG3   | 78:q2:71:ARG:NH1   | 2.23                     | 0.53              |
| 1:2:959:U:C6       | 15:C3:61:THR:HB    | 2.44                     | 0.53              |
| 1:2:1381:U:H1'     | 1:2:1516:A:N6      | 2.24                     | 0.53              |
| 6:S4:193:GLY:O     | 6:S4:194:THR:OG1   | 2.26                     | 0.53              |
| 10:S8:5:ARG:HD3    | 10:S8:29:LEU:O     | 2.07                     | 0.53              |
| 11:S9:118:LEU:HG   | 11:S9:158:PHE:CE1  | 2.44                     | 0.53              |
| 16:C4:16:VAL:HG22  | 16:C4:33:LEU:HA    | 1.90                     | 0.53              |
| 25:D3:92:CYS:HG    | 25:D3:136:TRP:CD1  | 2.26                     | 0.53              |
| 33:E1:136:LYS:O    | 33:E1:138:ARG:HB2  | 2.08                     | 0.53              |
| 36:1:567:G:O6      | 86:1:4006:OHX:N1   | 2.42                     | 0.53              |
| 36:1:786:A:H4'     | 36:1:787:G:H5'     | 1.89                     | 0.53              |
| 36:1:1245:A:H3'    | 36:1:1246:G:H5''   | 1.90                     | 0.53              |
| 36:1:1554:U:HO2'   | 36:1:1582:C:H5     | 1.56                     | 0.53              |
| 36:1:1577:G:H2'    | 36:1:1578:C:C1'    | 2.39                     | 0.53              |
| 86:1:4059:OHX:N4   | 86:1:4166:OHX:N1   | 2.56                     | 0.53              |
| 41:L4:152:VAL:CG2  | 41:L4:172:VAL:HG21 | 2.38                     | 0.53              |
| 42:L5:119:TYR:CZ   | 42:L5:135:VAL:HG23 | 2.44                     | 0.53              |
| 43:L6:52:VAL:HG11  | 43:L6:65:ILE:HG13  | 1.91                     | 0.53              |
| 47:M0:47:PRO:HB3   | 47:M0:171:TRP:CZ2  | 2.43                     | 0.53              |
| 57:N1:100:LYS:C    | 57:N1:102:ARG:H    | 2.15                     | 0.53              |
| 59:N3:80:ARG:NE    | 59:N3:97:ASP:OD2   | 2.40                     | 0.53              |
| 72:O6:53:TYR:HA    | 72:O6:56:ARG:NH1   | 2.24                     | 0.53              |
| 1:6:163:G:H8       | 1:6:163:G:O5'      | 1.92                     | 0.53              |
| 1:6:484:C:H42      | 1:6:503:G:H22      | 1.56                     | 0.53              |
| 8:s6:48:TYR:CZ     | 8:s6:121:LEU:HD22  | 2.43                     | 0.53              |
| 15:c3:71:ILE:O     | 15:c3:75:LEU:HD12  | 2.09                     | 0.53              |
| 36:5:961:C:O2      | 86:5:4176:OHX:N4   | 2.42                     | 0.53              |
| 36:5:2765:C:H2'    | 36:5:2766:U:C6     | 2.44                     | 0.53              |
| 38:8:38:U:H5       | 71:o5:82:ALA:O     | 1.92                     | 0.53              |
| 38:8:103:G:O6      | 86:8:216:OHX:N5    | 2.41                     | 0.53              |
| 86:8:215:OHX:N5    | 86:8:223:OHX:N1    | 2.57                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:l4:74:ILE:HD12  | 41:l4:75:PRO:HD2   | 1.91                     | 0.53              |
| 46:l9:174:LYS:HB2  | 76:q0:127:LEU:HD11 | 1.91                     | 0.53              |
| 63:n7:99:GLU:HG3   | 63:n7:100:THR:HG23 | 1.91                     | 0.53              |
| 69:o3:59:VAL:O     | 69:o3:61:GLY:N     | 2.41                     | 0.53              |
| 1:2:130:C:O2'      | 1:2:131:C:OP1      | 2.24                     | 0.53              |
| 1:2:703:G:H2'      | 1:2:704:C:H5'      | 1.90                     | 0.53              |
| 12:C0:55:VAL:HA    | 12:C0:69:THR:HG23  | 1.91                     | 0.53              |
| 18:C6:113:ASP:CG   | 18:C6:115:THR:H    | 2.17                     | 0.53              |
| 24:D2:103:ILE:HA   | 24:D2:112:ASP:HA   | 1.90                     | 0.53              |
| 26:D4:122:GLY:O    | 26:D4:125:LEU:N    | 2.35                     | 0.53              |
| 28:D6:18:VAL:HG21  | 28:D6:33:ASP:OD1   | 2.08                     | 0.53              |
| 51:M5:143:ARG:HH21 | 71:O5:92:LEU:HA    | 1.74                     | 0.53              |
| 57:N1:82:ASN:O     | 65:N9:21:ILE:HA    | 2.08                     | 0.53              |
| 57:N1:104:GLU:O    | 57:N1:108:ARG:HB2  | 2.09                     | 0.53              |
| 61:N5:136:ALA:O    | 61:N5:139:ILE:HG23 | 2.09                     | 0.53              |
| 1:6:1752:U:OP2     | 86:6:2061:OHX:N5   | 2.41                     | 0.53              |
| 11:s9:8:TYR:O      | 86:s9:201:OHX:N4   | 2.42                     | 0.53              |
| 15:c3:151:ASN:O    | 86:c3:201:OHX:N3   | 2.42                     | 0.53              |
| 36:5:1032:C:H5'    | 36:5:1033:U:OP2    | 2.09                     | 0.53              |
| 36:5:2771:U:O2'    | 36:5:2772:C:O5'    | 2.25                     | 0.53              |
| 36:5:2880:U:H1'    | 40:l3:250:ALA:HB3  | 1.91                     | 0.53              |
| 86:5:4201:OHX:N4   | 86:8:224:OHX:N1    | 2.56                     | 0.53              |
| 46:l9:12:VAL:HG13  | 46:l9:16:VAL:HG22  | 1.89                     | 0.53              |
| 48:m1:15:GLU:HB3   | 48:m1:130:VAL:HG22 | 1.89                     | 0.53              |
| 49:m3:128:ARG:NH1  | 71:o5:109:ILE:O    | 2.24                     | 0.53              |
| 49:m3:157:ARG:HH12 | 64:n8:146:GLU:CD   | 2.17                     | 0.53              |
| 61:n5:79:GLY:O     | 61:n5:81:ILE:HD12  | 2.09                     | 0.53              |
| 1:2:66:U:OP1       | 8:S6:136:LYS:NZ    | 2.34                     | 0.53              |
| 1:2:924:A:O2'      | 1:2:987:G:OP1      | 2.27                     | 0.53              |
| 1:2:1488:G:H5'     | 1:2:1489:U:OP1     | 2.09                     | 0.53              |
| 36:1:516:A:O3'     | 44:L7:60:ARG:NH2   | 2.40                     | 0.53              |
| 36:1:2303:A:OP1    | 77:Q1:23:ARG:NH2   | 2.41                     | 0.53              |
| 36:1:2402:A:O2'    | 36:1:2403:G:OP2    | 2.24                     | 0.53              |
| 36:1:2867:C:H5'    | 36:1:2867:C:C6     | 2.43                     | 0.53              |
| 42:L5:40:HIS:CD2   | 42:L5:42:ALA:H     | 2.18                     | 0.53              |
| 47:M0:4:ARG:CZ     | 47:M0:99:ILE:HD12  | 2.39                     | 0.53              |
| 51:M5:16:SER:O     | 51:M5:20:ARG:HG2   | 2.09                     | 0.53              |
| 2:s0:200:ASP:HA    | 2:s0:203:PHE:CE1   | 2.44                     | 0.53              |
| 3:s1:176:VAL:HG13  | 3:s1:184:LEU:HD22  | 1.91                     | 0.53              |
| 9:s7:9:LEU:HD21    | 9:s7:17:GLU:HB3    | 1.91                     | 0.53              |
| 13:c1:19:ILE:HD13  | 86:c1:202:OHX:N3   | 2.24                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:sR:197:SER:HB2 | 34:sR:216:LYS:HB3  | 1.91                     | 0.53              |
| 36:5:498:A:H5'    | 69:o3:86:ARG:HH12  | 1.74                     | 0.53              |
| 36:5:1317:A:OP1   | 86:5:4097:OHX:N1   | 2.42                     | 0.53              |
| 36:5:2177:G:OP2   | 39:l2:128:ARG:NH1  | 2.40                     | 0.53              |
| 86:5:4212:OHX:N4  | 86:5:4222:OHX:N3   | 2.56                     | 0.53              |
| 37:7:3:U:H2'      | 37:7:4:U:H6        | 1.72                     | 0.53              |
| 38:8:38:U:C4      | 71:o5:89:ARG:HD2   | 2.44                     | 0.53              |
| 62:n6:37:LYS:H    | 62:n6:37:LYS:CE    | 2.22                     | 0.53              |
| 1:2:839:U:C2'     | 1:2:840:U:H5'      | 2.39                     | 0.53              |
| 1:2:1235:C:C2     | 33:E1:138:ARG:NH2  | 2.77                     | 0.53              |
| 3:S1:131:ASP:HB3  | 3:S1:180:THR:HG23  | 1.91                     | 0.53              |
| 7:S5:94:THR:HB    | 7:S5:114:ILE:HG13  | 1.91                     | 0.53              |
| 9:S7:14:THR:OG1   | 9:S7:15:GLU:N      | 2.41                     | 0.53              |
| 12:C0:16:PHE:HD2  | 12:C0:76:LEU:HD23  | 1.74                     | 0.53              |
| 15:C3:37:ILE:HD13 | 15:C3:74:ILE:HD13  | 1.91                     | 0.53              |
| 24:D2:37:PHE:CD2  | 24:D2:103:ILE:HD12 | 2.44                     | 0.53              |
| 28:D6:10:ARG:HB3  | 28:D6:34:LYS:HA    | 1.90                     | 0.53              |
| 86:1:3943:OHX:N1  | 86:1:4200:OHX:N2   | 2.57                     | 0.53              |
| 38:4:85:G:O6      | 62:N6:112:ASP:HB3  | 2.09                     | 0.53              |
| 42:L5:226:TYR:HE2 | 42:L5:236:LEU:HD11 | 1.74                     | 0.53              |
| 50:M4:92:GLU:OE2  | 50:M4:92:GLU:N     | 2.35                     | 0.53              |
| 59:N3:129:VAL:O   | 59:N3:133:SER:OG   | 2.26                     | 0.53              |
| 62:N6:47:ALA:O    | 62:N6:122:LYS:NZ   | 2.42                     | 0.53              |
| 1:6:727:U:H2'     | 1:6:728:U:H6       | 1.73                     | 0.53              |
| 1:6:1584:G:H22    | 1:6:1611:A:P       | 2.31                     | 0.53              |
| 2:s0:168:HIS:HB3  | 2:s0:203:PHE:CZ    | 2.44                     | 0.53              |
| 7:s5:43:PHE:HB3   | 7:s5:46:TRP:HD1    | 1.74                     | 0.53              |
| 10:s8:8:ARG:HH21  | 10:s8:22:ARG:NH1   | 2.07                     | 0.53              |
| 11:s9:162:SER:O   | 11:s9:165:GLY:N    | 2.42                     | 0.53              |
| 17:c5:51:SER:C    | 17:c5:53:PRO:HD2   | 2.34                     | 0.53              |
| 24:d2:41:MET:HG2  | 24:d2:129:VAL:HG21 | 1.91                     | 0.53              |
| 36:5:790:U:H4'    | 41:l4:112:LYS:HG2  | 1.90                     | 0.53              |
| 36:5:1237:G:H22   | 36:5:1251:A:H2     | 1.57                     | 0.53              |
| 43:l6:47:PHE:CD1  | 43:l6:74:VAL:HG22  | 2.43                     | 0.53              |
| 44:l7:73:GLY:O    | 57:n1:143:THR:HB   | 2.09                     | 0.53              |
| 51:m5:5:LYS:NZ    | 51:m5:8:GLU:OE1    | 2.41                     | 0.53              |
| 52:m6:171:LYS:O   | 52:m6:175:THR:HG22 | 2.09                     | 0.53              |
| 53:m7:67:ILE:HD12 | 53:m7:82:ARG:CZ    | 2.39                     | 0.53              |
| 58:n2:22:PRO:HB2  | 58:n2:28:PHE:HB2   | 1.90                     | 0.53              |
| 1:2:1258:U:H4'    | 12:C0:2:LEU:HD13   | 1.91                     | 0.52              |
| 2:S0:147:THR:OG1  | 2:S0:159:ALA:HB1   | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:S0:167:LYS:HG2   | 2:S0:168:HIS:CE1  | 2.44                     | 0.52              |
| 11:S9:163:PRO:C    | 11:S9:165:GLY:H   | 2.14                     | 0.52              |
| 14:C2:55:GLY:HA2   | 14:C2:85:LYS:HE3  | 1.90                     | 0.52              |
| 36:1:535:G:O6      | 86:1:4064:OHX:N3  | 2.41                     | 0.52              |
| 36:1:926:A:H2'     | 36:1:927:C:C6     | 2.44                     | 0.52              |
| 36:1:3294:A:H2'    | 36:1:3295:A:O4'   | 2.09                     | 0.52              |
| 42:L5:58:LYS:HD2   | 42:L5:93:THR:HG21 | 1.89                     | 0.52              |
| 42:L5:261:THR:HG23 | 42:L5:264:GLN:NE2 | 2.23                     | 0.52              |
| 45:L8:71:VAL:HG22  | 45:L8:76:ALA:HB2  | 1.91                     | 0.52              |
| 48:M1:12:LEU:HD12  | 48:M1:131:MET:HE3 | 1.91                     | 0.52              |
| 49:M3:124:ILE:HD11 | 49:M3:126:PHE:CZ  | 2.44                     | 0.52              |
| 51:M5:184:LYS:H    | 51:M5:186:GLY:H   | 1.54                     | 0.52              |
| 55:M9:96:ILE:O     | 55:M9:100:ARG:HG3 | 2.09                     | 0.52              |
| 67:O1:13:THR:HG22  | 67:O1:72:ARG:CD   | 2.40                     | 0.52              |
| 1:6:753:A:H62      | 6:s4:187:ARG:NH2  | 2.07                     | 0.52              |
| 1:6:1330:G:N2      | 19:c7:8:THR:HG21  | 2.16                     | 0.52              |
| 2:s0:175:TYR:HE1   | 2:s0:197:ILE:HG22 | 1.74                     | 0.52              |
| 11:s9:146:PHE:O    | 11:s9:147:MET:HB2 | 2.09                     | 0.52              |
| 20:c8:42:TYR:HE2   | 20:c8:73:MET:HG3  | 1.74                     | 0.52              |
| 34:sR:38:ARG:HA    | 34:sR:67:ILE:HG23 | 1.91                     | 0.52              |
| 36:5:1716:U:H5'    | 36:5:1716:U:C6    | 2.43                     | 0.52              |
| 36:5:2397:A:C2     | 36:5:2873:U:H5'   | 2.44                     | 0.52              |
| 37:7:64:A:N1       | 47:m0:202:LYS:HD3 | 2.23                     | 0.52              |
| 41:l4:290:ILE:HG23 | 54:m8:35:PHE:CE2  | 2.44                     | 0.52              |
| 57:n1:12:ARG:HD3   | 57:n1:13:TYR:CZ   | 2.44                     | 0.52              |
| 69:o3:59:VAL:HG23  | 69:o3:60:ARG:N    | 2.24                     | 0.52              |
| 1:2:108:A:H2'      | 1:2:109:G:C8      | 2.45                     | 0.52              |
| 1:2:959:U:H5'      | 29:D7:28:PRO:HB3  | 1.92                     | 0.52              |
| 1:2:992:A:H2       | 1:2:1012:U:N3     | 2.01                     | 0.52              |
| 2:S0:163:ASN:C     | 2:S0:165:ARG:H    | 2.17                     | 0.52              |
| 4:S2:203:LYS:O     | 4:S2:206:THR:HG23 | 2.08                     | 0.52              |
| 9:S7:44:LYS:HZ2    | 9:S7:95:GLU:HG2   | 1.74                     | 0.52              |
| 15:C3:23:PRO:O     | 15:C3:25:TRP:N    | 2.42                     | 0.52              |
| 22:D0:67:THR:HG21  | 31:D9:40:ARG:HB2  | 1.90                     | 0.52              |
| 26:D4:35:VAL:O     | 26:D4:36:SER:HB3  | 2.09                     | 0.52              |
| 36:1:304:G:H5'     | 36:1:304:G:N3     | 2.24                     | 0.52              |
| 36:1:2097:U:H2'    | 36:1:2098:C:C6    | 2.44                     | 0.52              |
| 86:1:4208:OHX:N4   | 38:4:16:G:OP1     | 2.42                     | 0.52              |
| 40:L3:331:ASN:N    | 40:L3:331:ASN:OD1 | 2.38                     | 0.52              |
| 61:N5:80:ASN:ND2   | 61:N5:126:LEU:HB2 | 2.24                     | 0.52              |
| 79:Q3:37:TYR:HB2   | 79:Q3:47:VAL:HB   | 1.91                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:6:946:U:H2'     | 1:6:947:U:C6       | 2.44                     | 0.52              |
| 1:6:1133:A:H2'    | 1:6:1134:C:O4'     | 2.09                     | 0.52              |
| 8:s6:67:VAL:HG21  | 8:s6:99:GLY:HA2    | 1.89                     | 0.52              |
| 23:d1:71:ARG:HG3  | 23:d1:83:TRP:CZ2   | 2.43                     | 0.52              |
| 36:5:252:U:H4'    | 36:5:253:A:C5'     | 2.40                     | 0.52              |
| 36:5:1754:G:OP1   | 86:5:4076:OHX:N1   | 2.42                     | 0.52              |
| 36:5:1831:U:OP2   | 61:n5:92:LYS:HD2   | 2.09                     | 0.52              |
| 36:5:2112:U:H4'   | 36:5:2113:A:H5'    | 1.91                     | 0.52              |
| 36:5:3150:A:H5'   | 40:l3:129:ALA:O    | 2.09                     | 0.52              |
| 86:5:4011:OHX:N6  | 86:5:4198:OHX:N5   | 2.57                     | 0.52              |
| 86:5:4094:OHX:N1  | 86:5:4234:OHX:N4   | 2.57                     | 0.52              |
| 40:l3:92:TYR:O    | 40:l3:155:ALA:HA   | 2.08                     | 0.52              |
| 59:n3:13:ILE:HG12 | 59:n3:53:SER:HB2   | 1.92                     | 0.52              |
| 1:2:144:U:H5      | 8:S6:137:ARG:NH1   | 2.07                     | 0.52              |
| 1:2:629:U:OP1     | 15:C3:127:ARG:NH2  | 2.42                     | 0.52              |
| 1:2:767:U:H5      | 11:S9:142:ASN:OD1  | 1.91                     | 0.52              |
| 3:S1:173:THR:O    | 3:S1:177:GLN:NE2   | 2.42                     | 0.52              |
| 25:D3:50:LYS:HD3  | 25:D3:101:GLU:HG2  | 1.91                     | 0.52              |
| 36:1:239:G:O6     | 86:1:4038:OHX:N3   | 2.42                     | 0.52              |
| 36:1:830:A:H2'    | 36:1:831:G:O4'     | 2.09                     | 0.52              |
| 36:1:1688:U:H2'   | 36:1:1689:U:C6     | 2.45                     | 0.52              |
| 36:1:3278:C:H2'   | 36:1:3278:C:O2     | 2.07                     | 0.52              |
| 42:L5:4:GLN:H     | 42:L5:4:GLN:CD     | 2.17                     | 0.52              |
| 44:L7:24:GLU:O    | 44:L7:26:VAL:N     | 2.30                     | 0.52              |
| 45:L8:161:GLU:HA  | 45:L8:164:VAL:HG22 | 1.90                     | 0.52              |
| 52:M6:88:VAL:O    | 52:M6:90:HIS:N     | 2.43                     | 0.52              |
| 62:N6:112:ASP:HB2 | 62:N6:115:ARG:H    | 1.75                     | 0.52              |
| 3:s1:129:THR:OG1  | 3:s1:131:ASP:O     | 2.28                     | 0.52              |
| 22:d0:105:GLN:HA  | 22:d0:108:ILE:HD13 | 1.90                     | 0.52              |
| 25:d3:37:ALA:O    | 25:d3:41:SER:HB3   | 2.09                     | 0.52              |
| 27:d5:61:SER:H    | 27:d5:64:VAL:HB    | 1.74                     | 0.52              |
| 36:5:629:U:H2'    | 36:5:630:A:C8      | 2.45                     | 0.52              |
| 36:5:1330:A:OP1   | 69:o3:19:SER:HB3   | 2.09                     | 0.52              |
| 36:5:1560:G:H2'   | 36:5:1561:G:C8     | 2.44                     | 0.52              |
| 36:5:2746:A:H2'   | 36:5:2747:A:O4'    | 2.10                     | 0.52              |
| 36:5:3027:A:H2'   | 36:5:3028:G:O4'    | 2.10                     | 0.52              |
| 37:7:121:U:H5''   | 42:l5:265:TYR:HE1  | 1.73                     | 0.52              |
| 38:8:77:A:H2'     | 38:8:78:G:O4'      | 2.10                     | 0.52              |
| 53:m7:59:PRO:HG3  | 53:m7:76:PHE:CD1   | 2.45                     | 0.52              |
| 1:2:482:U:H2'     | 1:2:483:A:C8       | 2.44                     | 0.52              |
| 1:2:581:U:OP2     | 5:S3:143:ARG:NH1   | 2.42                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1102:G:OP2     | 25:D3:7:ARG:NH1    | 2.43                     | 0.52              |
| 1:2:1492:A:HO2'    | 1:2:1493:A:H8      | 1.56                     | 0.52              |
| 1:2:1588:G:OP1     | 86:2:2117:OHX:N3   | 2.42                     | 0.52              |
| 7:S5:40:ILE:HG23   | 7:S5:42:LEU:HD22   | 1.92                     | 0.52              |
| 8:S6:109:LEU:HD13  | 8:S6:111:LEU:HD21  | 1.90                     | 0.52              |
| 16:C4:122:PRO:O    | 16:C4:124:ASP:N    | 2.43                     | 0.52              |
| 23:D1:1:MET:HE3    | 23:D1:10:GLU:O     | 2.10                     | 0.52              |
| 29:D7:61:THR:HG23  | 29:D7:62:ILE:O     | 2.08                     | 0.52              |
| 36:1:2401:A:O2'    | 41:L4:68:GLY:HA2   | 2.09                     | 0.52              |
| 36:1:2617:U:H5     | 36:1:2621:G:OP2    | 1.93                     | 0.52              |
| 36:1:2697:A:H2'    | 36:1:2698:G:H8     | 1.74                     | 0.52              |
| 36:1:3308:C:O2     | 53:M7:69:ARG:HD3   | 2.10                     | 0.52              |
| 86:1:3955:OHX:N4   | 86:1:4041:OHX:N5   | 2.58                     | 0.52              |
| 86:1:4007:OHX:N6   | 86:1:4175:OHX:N5   | 2.56                     | 0.52              |
| 51:M5:155:VAL:O    | 51:M5:162:ARG:NH2  | 2.38                     | 0.52              |
| 1:6:169:A:C5'      | 8:s6:176:GLN:HG2   | 2.39                     | 0.52              |
| 1:6:653:C:H42      | 1:6:677:G:H1       | 1.56                     | 0.52              |
| 1:6:1572:G:H2'     | 1:6:1572:G:N3      | 2.24                     | 0.52              |
| 2:s0:140:ASN:HD22  | 4:s2:62:PRO:HD3    | 1.73                     | 0.52              |
| 6:s4:117:GLU:O     | 6:s4:119:ALA:N     | 2.34                     | 0.52              |
| 12:c0:49:LEU:HB3   | 12:c0:55:VAL:CG1   | 2.40                     | 0.52              |
| 29:d7:81:ARG:O     | 29:d7:82:LYS:HE3   | 2.07                     | 0.52              |
| 36:5:112:U:O2'     | 36:5:113:C:OP2     | 2.27                     | 0.52              |
| 36:5:181:U:H1'     | 36:5:236:G:N2      | 2.25                     | 0.52              |
| 36:5:683:U:H5''    | 51:m5:200:TRP:CE3  | 2.44                     | 0.52              |
| 36:5:3189:G:H2'    | 36:5:3190:C:O4'    | 2.09                     | 0.52              |
| 36:5:3379:C:H4'    | 40:l3:315:GLY:HA2  | 1.92                     | 0.52              |
| 86:5:4011:OHX:N4   | 86:5:4198:OHX:N1   | 2.57                     | 0.52              |
| 40:l3:150:ARG:HG2  | 40:l3:150:ARG:HH11 | 1.75                     | 0.52              |
| 46:l9:8:GLN:NE2    | 46:l9:69:ARG:HG2   | 2.24                     | 0.52              |
| 63:n7:5:LEU:HD23   | 63:n7:25:ILE:HD13  | 1.90                     | 0.52              |
| 65:n9:16:ALA:O     | 65:n9:20:GLY:HA3   | 2.09                     | 0.52              |
| 70:o4:81:CYS:O     | 70:o4:81:CYS:SG    | 2.67                     | 0.52              |
| 1:2:1585:U:N3      | 1:2:1611:A:C2      | 2.69                     | 0.52              |
| 2:S0:175:TYR:HE1   | 2:S0:197:ILE:HG22  | 1.75                     | 0.52              |
| 6:S4:19:LEU:HD11   | 6:S4:108:ARG:HD2   | 1.90                     | 0.52              |
| 11:S9:96:VAL:HA    | 11:S9:99:LEU:HD22  | 1.92                     | 0.52              |
| 14:C2:61:VAL:HA    | 14:C2:89:ILE:HG22  | 1.91                     | 0.52              |
| 21:C9:117:SER:OG   | 21:C9:118:PRO:O    | 2.27                     | 0.52              |
| 34:SR:116:ASP:HB2  | 34:SR:117:LYS:HD2  | 1.92                     | 0.52              |
| 34:SR:211:ILE:HG22 | 34:SR:223:TRP:CD1  | 2.42                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:316:U:O2'    | 72:O6:30:LYS:HD2   | 2.08                     | 0.52              |
| 36:1:929:A:H2'    | 36:1:930:U:C6      | 2.45                     | 0.52              |
| 36:1:1528:G:O2'   | 36:1:1588:A:N3     | 2.41                     | 0.52              |
| 36:1:2403:G:H22   | 36:1:2404:A:H62    | 1.57                     | 0.52              |
| 36:1:2440:G:H1    | 36:1:2507:C:H42    | 1.58                     | 0.52              |
| 36:1:2895:G:O2'   | 76:Q0:100:TYR:O    | 2.24                     | 0.52              |
| 36:1:2976:A:OP1   | 86:1:4123:OHX:N6   | 2.43                     | 0.52              |
| 36:1:3185:U:C6    | 52:M6:126:VAL:HG21 | 2.44                     | 0.52              |
| 36:1:3275:U:H5''  | 69:O3:68:TRP:HZ2   | 1.74                     | 0.52              |
| 86:1:3964:OHX:N1  | 86:1:4143:OHX:N3   | 2.58                     | 0.52              |
| 86:1:4036:OHX:N6  | 86:1:4048:OHX:N5   | 2.58                     | 0.52              |
| 48:M1:21:ILE:HG22 | 48:M1:23:VAL:HG22  | 1.91                     | 0.52              |
| 49:M3:64:LYS:HD3  | 49:M3:65:TYR:CE1   | 2.44                     | 0.52              |
| 58:N2:33:TYR:CE2  | 58:N2:63:VAL:HG21  | 2.45                     | 0.52              |
| 60:N4:52:THR:O    | 60:N4:56:ARG:HG3   | 2.10                     | 0.52              |
| 61:N5:100:LYS:NZ  | 61:N5:106:ASP:OD2  | 2.37                     | 0.52              |
| 2:s0:118:PRO:HG2  | 2:s0:141:ILE:HD13  | 1.90                     | 0.52              |
| 7:s5:188:LYS:HD2  | 7:s5:193:THR:HG22  | 1.90                     | 0.52              |
| 31:d9:4:GLU:OE2   | 33:e1:145:HIS:NE2  | 2.42                     | 0.52              |
| 36:5:247:C:C2     | 36:5:248:U:H1'     | 2.44                     | 0.52              |
| 36:5:549:U:O4     | 86:5:4013:OHX:N4   | 2.43                     | 0.52              |
| 36:5:1276:U:OP2   | 86:5:4007:OHX:N1   | 2.43                     | 0.52              |
| 36:5:1307:G:C2    | 36:5:1308:A:C2     | 2.97                     | 0.52              |
| 36:5:2725:U:O4    | 86:5:3959:OHX:N1   | 2.42                     | 0.52              |
| 55:m9:154:ALA:O   | 55:m9:156:ASN:N    | 2.38                     | 0.52              |
| 71:o5:44:ILE:O    | 71:o5:48:ARG:HG3   | 2.09                     | 0.52              |
| 78:q2:17:CYS:SG   | 78:q2:77:CYS:CB    | 2.77                     | 0.52              |
| 1:2:692:C:H2'     | 1:2:693:U:O4'      | 2.10                     | 0.52              |
| 1:2:1657:U:C2     | 86:2:2090:OHX:N1   | 2.78                     | 0.52              |
| 1:2:1672:G:H2'    | 1:2:1673:G:C8      | 2.44                     | 0.52              |
| 86:2:2045:OHX:N2  | 86:2:2099:OHX:N5   | 2.58                     | 0.52              |
| 86:1:4036:OHX:N2  | 86:1:4048:OHX:N1   | 2.57                     | 0.52              |
| 39:L2:83:HIS:CE1  | 39:L2:86:GLN:HB2   | 2.44                     | 0.52              |
| 48:M1:40:LEU:HD23 | 48:M1:114:ILE:HD11 | 1.92                     | 0.52              |
| 49:M3:87:ALA:O    | 49:M3:91:ARG:HG3   | 2.10                     | 0.52              |
| 50:M4:48:GLY:HA3  | 50:M4:53:VAL:HG13  | 1.92                     | 0.52              |
| 51:M5:91:GLU:O    | 51:M5:93:LYS:HE3   | 2.08                     | 0.52              |
| 59:N3:11:PHE:CG   | 59:N3:88:ARG:HD2   | 2.44                     | 0.52              |
| 70:O4:99:LYS:O    | 70:O4:103:LYS:HG2  | 2.10                     | 0.52              |
| 1:6:1071:U:H2'    | 1:6:1072:C:C6      | 2.44                     | 0.52              |
| 1:6:1756:A:O5'    | 1:6:1756:A:H8      | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:s0:56:LYS:HE2    | 2:s0:159:ALA:O     | 2.09                     | 0.52              |
| 4:s2:56:ILE:HG23   | 4:s2:61:LEU:HB2    | 1.92                     | 0.52              |
| 15:c3:132:VAL:HG23 | 15:c3:134:VAL:HG13 | 1.91                     | 0.52              |
| 22:d0:36:ASN:HA    | 22:d0:39:SER:HB2   | 1.92                     | 0.52              |
| 25:d3:100:ASP:O    | 25:d3:101:GLU:HB3  | 2.09                     | 0.52              |
| 36:5:77:A:N7       | 49:m3:73:ARG:NH2   | 2.58                     | 0.52              |
| 36:5:621:A:H2'     | 36:5:622:A:C8      | 2.45                     | 0.52              |
| 36:5:2155:G:OP1    | 39:l2:241:ARG:HG2  | 2.09                     | 0.52              |
| 36:5:2562:A:N6     | 36:5:2579:G:O2'    | 2.41                     | 0.52              |
| 36:5:2567:C:N4     | 36:5:2568:C:H41    | 2.08                     | 0.52              |
| 36:5:3227:A:C2'    | 36:5:3228:C:H5'    | 2.40                     | 0.52              |
| 86:5:4001:OHX:N2   | 77:q1:23:ARG:O     | 2.43                     | 0.52              |
| 41:l4:204:GLY:O    | 41:l4:246:ARG:NH1  | 2.38                     | 0.52              |
| 57:n1:32:LYS:NZ    | 57:n1:98:HIS:H     | 2.08                     | 0.52              |
| 3:S1:29:TRP:CD1    | 3:S1:47:LEU:HG     | 2.44                     | 0.52              |
| 9:S7:58:LEU:HG     | 9:S7:88:ARG:HD2    | 1.91                     | 0.52              |
| 10:S8:105:ASP:O    | 10:S8:107:THR:N    | 2.38                     | 0.52              |
| 14:C2:118:ALA:O    | 14:C2:120:VAL:N    | 2.43                     | 0.52              |
| 21:C9:86:ARG:HH11  | 21:C9:86:ARG:HG3   | 1.75                     | 0.52              |
| 23:D1:81:ASN:O     | 23:D1:82:VAL:HB    | 2.10                     | 0.52              |
| 36:1:789:A:H2'     | 36:1:790:U:C6      | 2.45                     | 0.52              |
| 36:1:1845:G:O2'    | 73:O7:5:THR:HB     | 2.10                     | 0.52              |
| 36:1:3095:U:H2'    | 36:1:3096:C:C6     | 2.44                     | 0.52              |
| 40:L3:60:LEU:HD23  | 40:L3:67:PHE:HB3   | 1.92                     | 0.52              |
| 1:6:315:A:O2'      | 86:6:2160:OHX:N1   | 2.43                     | 0.52              |
| 1:6:485:A:C6       | 1:6:486:G:H1'      | 2.45                     | 0.52              |
| 1:6:567:A:H4'      | 80:e0:13:LYS:HB2   | 1.91                     | 0.52              |
| 4:s2:88:LYS:HD3    | 4:s2:89:GLN:O      | 2.09                     | 0.52              |
| 14:c2:103:LEU:HG   | 14:c2:116:VAL:HG13 | 1.92                     | 0.52              |
| 23:d1:40:ASP:OD1   | 23:d1:44:ARG:HB2   | 2.10                     | 0.52              |
| 26:d4:15:ASN:OD1   | 26:d4:17:LEU:HB2   | 2.10                     | 0.52              |
| 29:d7:36:LYS:HB3   | 29:d7:42:ASN:O     | 2.10                     | 0.52              |
| 36:5:437:G:H5''    | 36:5:438:A:OP2     | 2.09                     | 0.52              |
| 36:5:1246:G:O2'    | 36:5:1264:G:OP2    | 2.28                     | 0.52              |
| 36:5:2549:G:C2     | 45:l8:33:ASN:HA    | 2.44                     | 0.52              |
| 36:5:2875:U:H5     | 36:5:2945:G:O6     | 1.92                     | 0.52              |
| 36:5:3279:A:C2'    | 36:5:3280:U:H5'    | 2.40                     | 0.52              |
| 86:5:4066:OHX:N1   | 86:5:4141:OHX:N2   | 2.58                     | 0.52              |
| 56:n0:42:TRP:O     | 56:n0:46:GLN:HG3   | 2.09                     | 0.52              |
| 1:2:192:U:O2'      | 1:2:193:U:O5'      | 2.27                     | 0.52              |
| 1:2:840:U:O2'      | 1:2:841:U:H5''     | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:1488:G:H3'    | 1:2:1515:A:H61     | 1.74                     | 0.52              |
| 1:2:1657:U:C4     | 86:2:2090:OHX:N4   | 2.78                     | 0.52              |
| 3:S1:104:ASP:HA   | 3:S1:214:LYS:HE2   | 1.92                     | 0.52              |
| 5:S3:20:GLU:HG3   | 12:C0:61:TRP:CD2   | 2.45                     | 0.52              |
| 6:S4:156:VAL:O    | 6:S4:157:ASN:HB2   | 2.10                     | 0.52              |
| 18:C6:82:ARG:HH12 | 18:C6:114:ARG:HB3  | 1.75                     | 0.52              |
| 24:D2:37:PHE:CE2  | 24:D2:103:ILE:HD12 | 2.45                     | 0.52              |
| 28:D6:49:ALA:O    | 28:D6:53:LEU:N     | 2.42                     | 0.52              |
| 36:1:121:A:C2     | 45:L8:129:PRO:HB3  | 2.45                     | 0.52              |
| 36:1:662:U:H2'    | 36:1:663:C:C6      | 2.45                     | 0.52              |
| 36:1:1540:U:OP1   | 86:1:4023:OHX:N1   | 2.42                     | 0.52              |
| 36:1:2415:C:OP1   | 39:L2:2:GLY:HA2    | 2.10                     | 0.52              |
| 36:1:2528:G:N7    | 86:1:4186:OHX:N3   | 2.57                     | 0.52              |
| 36:1:2698:G:O2'   | 57:N1:12:ARG:HG3   | 2.10                     | 0.52              |
| 41:L4:144:LYS:HA  | 86:L4:404:OHX:N2   | 2.25                     | 0.52              |
| 61:N5:73:MET:HE1  | 61:N5:141:TYR:HE1  | 1.75                     | 0.52              |
| 73:O7:22:CYS:SG   | 73:O7:24:ARG:HB2   | 2.49                     | 0.52              |
| 76:Q0:94:SER:HB2  | 76:Q0:122:ARG:O    | 2.09                     | 0.52              |
| 78:Q2:3:ASN:HB2   | 78:Q2:92:GLU:HG3   | 1.92                     | 0.52              |
| 1:6:193:U:C4      | 1:6:195:G:C8       | 2.98                     | 0.52              |
| 1:6:488:G:N2      | 1:6:499:U:H3       | 2.07                     | 0.52              |
| 1:6:765:G:N7      | 11:s9:149:ARG:NE   | 2.58                     | 0.52              |
| 9:s7:89:HIS:CD2   | 9:s7:165:LYS:HG2   | 2.45                     | 0.52              |
| 29:d7:47:PHE:CE1  | 29:d7:49:HIS:HB2   | 2.45                     | 0.52              |
| 86:5:4055:OHX:N3  | 86:5:4197:OHX:N4   | 2.57                     | 0.52              |
| 42:l5:120:LYS:NZ  | 42:l5:123:GLU:OE1  | 2.32                     | 0.52              |
| 44:l7:228:SER:HA  | 44:l7:232:ARG:NH2  | 2.25                     | 0.52              |
| 46:l9:162:GLN:HG3 | 46:l9:163:GLN:N    | 2.25                     | 0.52              |
| 55:m9:4:LEU:O     | 55:m9:7:GLN:HG2    | 2.10                     | 0.52              |
| 61:n5:38:LEU:O    | 61:n5:39:LYS:HB2   | 2.08                     | 0.52              |
| 65:n9:5:LYS:HE2   | 65:n9:8:THR:HB     | 1.92                     | 0.52              |
| 1:2:93:A:O2'      | 6:S4:4:GLY:HA3     | 2.10                     | 0.52              |
| 11:S9:83:VAL:HG23 | 11:S9:85:VAL:HG23  | 1.92                     | 0.52              |
| 14:C2:40:GLY:HA3  | 14:C2:125:ASN:HB3  | 1.91                     | 0.52              |
| 20:C8:6:GLN:O     | 27:D5:42:LEU:HD13  | 2.10                     | 0.52              |
| 21:C9:6:VAL:HG13  | 21:C9:66:TYR:CE1   | 2.45                     | 0.52              |
| 35:SM:97:THR:C    | 35:SM:99:LYS:H     | 2.18                     | 0.52              |
| 36:1:114:A:N1     | 36:1:266:A:O2'     | 2.39                     | 0.52              |
| 36:1:530:G:N7     | 86:1:3924:OHX:N6   | 2.58                     | 0.52              |
| 36:1:1507:G:H5'   | 36:1:1507:G:N3     | 2.24                     | 0.52              |
| 36:1:3228:C:O2'   | 36:1:3229:G:OP2    | 2.26                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:3:3:U:H2'       | 37:3:4:U:C6        | 2.45                     | 0.52              |
| 39:L2:13:GLY:HA2   | 39:L2:16:PHE:HB2   | 1.92                     | 0.52              |
| 42:L5:113:LEU:HB3  | 42:L5:115:LEU:HD22 | 1.91                     | 0.52              |
| 45:L8:67:ILE:CG2   | 45:L8:237:ILE:HD12 | 2.40                     | 0.52              |
| 73:O7:28:HIS:ND1   | 73:O7:31:LYS:HB2   | 2.25                     | 0.52              |
| 1:6:248:U:OP1      | 86:6:2123:OHX:N3   | 2.43                     | 0.52              |
| 1:6:425:A:H5'      | 1:6:425:A:H8       | 1.75                     | 0.52              |
| 3:s1:62:LYS:O      | 3:s1:88:VAL:HB     | 2.10                     | 0.52              |
| 4:s2:186:LYS:HD2   | 4:s2:189:GLN:OE1   | 2.09                     | 0.52              |
| 20:c8:31:ALA:O     | 20:c8:34:THR:HG22  | 2.09                     | 0.52              |
| 36:5:1095:U:N3     | 57:n1:127:GLN:HG3  | 2.23                     | 0.52              |
| 36:5:1414:G:O6     | 86:5:4145:OHX:N1   | 2.43                     | 0.52              |
| 36:5:1778:G:O2'    | 36:5:1780:G:OP2    | 2.26                     | 0.52              |
| 36:5:2841:G:OP2    | 86:5:4136:OHX:N1   | 2.43                     | 0.52              |
| 37:7:77:G:N2       | 37:7:102:A:OP2     | 2.36                     | 0.52              |
| 40:l3:221:THR:HG22 | 40:l3:273:HIS:H    | 1.73                     | 0.52              |
| 40:l3:238:LEU:HB3  | 40:l3:242:THR:HG21 | 1.92                     | 0.52              |
| 43:l6:47:PHE:O     | 43:l6:50:LYS:HB2   | 2.09                     | 0.52              |
| 44:l7:27:ALA:HA    | 44:l7:30:ARG:HB3   | 1.92                     | 0.52              |
| 1:2:1283:U:OP1     | 86:2:2115:OHX:N2   | 2.42                     | 0.52              |
| 1:2:1487:A:H2'     | 1:2:1488:G:C8      | 2.45                     | 0.52              |
| 7:S5:145:ASP:OD2   | 7:S5:146:THR:N     | 2.43                     | 0.52              |
| 8:S6:19:ASP:O      | 8:S6:20:ASP:HB2    | 2.10                     | 0.52              |
| 8:S6:78:THR:HG23   | 8:S6:92:ARG:HG2    | 1.92                     | 0.52              |
| 19:C7:99:VAL:CB    | 19:C7:118:PRO:HB2  | 2.40                     | 0.52              |
| 22:D0:57:ARG:HG3   | 22:D0:89:ARG:CZ    | 2.40                     | 0.52              |
| 36:1:671:U:OP2     | 54:M8:57:ILE:HD12  | 2.10                     | 0.52              |
| 36:1:3206:C:O2     | 56:N0:155:ARG:NH1  | 2.43                     | 0.52              |
| 62:N6:56:VAL:HG11  | 62:N6:104:LEU:HD13 | 1.91                     | 0.52              |
| 73:O7:31:LYS:O     | 73:O7:33:THR:HG22  | 2.10                     | 0.52              |
| 1:6:93:A:H1'       | 6:s4:3:ARG:HB3     | 1.92                     | 0.52              |
| 1:6:166:C:OP2      | 86:6:2170:OHX:N4   | 2.43                     | 0.52              |
| 4:s2:179:VAL:O     | 4:s2:198:THR:OG1   | 2.20                     | 0.52              |
| 36:5:252:U:H4'     | 36:5:253:A:H5'     | 1.92                     | 0.52              |
| 36:5:900:G:H1'     | 36:5:1589:A:N6     | 2.25                     | 0.52              |
| 36:5:999:G:O2'     | 36:5:1000:C:H5'    | 2.09                     | 0.52              |
| 36:5:1812:G:O6     | 63:n7:64:LYS:HD2   | 2.10                     | 0.52              |
| 36:5:3294:A:H2'    | 36:5:3295:A:O4'    | 2.10                     | 0.52              |
| 44:l7:229:PHE:CD1  | 44:l7:229:PHE:C    | 2.88                     | 0.52              |
| 55:m9:43:LYS:HD2   | 55:m9:43:LYS:N     | 2.24                     | 0.52              |
| 55:m9:154:ALA:O    | 55:m9:158:GLU:HG2  | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:n7:27:LYS:HB3  | 63:n7:42:LEU:HB2   | 1.91                     | 0.52              |
| 69:o3:23:ASN:OD1  | 69:o3:25:PRO:HD3   | 2.10                     | 0.52              |
| 73:o7:48:ASN:HA   | 73:o7:54:LYS:NZ    | 2.25                     | 0.52              |
| 1:2:416:A:H5'     | 1:2:417:A:N7       | 2.25                     | 0.51              |
| 1:2:730:G:H21     | 1:2:731:C:H5'      | 1.75                     | 0.51              |
| 1:2:1774:G:N7     | 77:Q1:4:LYS:NZ     | 2.58                     | 0.51              |
| 9:S7:131:PHE:HB3  | 9:S7:132:PRO:CD    | 2.41                     | 0.51              |
| 23:D1:40:ASP:OD2  | 23:D1:44:ARG:NH2   | 2.43                     | 0.51              |
| 27:D5:50:ILE:HG22 | 27:D5:51:LEU:HD12  | 1.91                     | 0.51              |
| 28:D6:79:ILE:HA   | 28:D6:84:VAL:CB    | 2.37                     | 0.51              |
| 36:1:1478:C:H2'   | 36:1:1479:U:C6     | 2.44                     | 0.51              |
| 36:1:1765:U:OP1   | 36:1:1765:U:H4'    | 2.10                     | 0.51              |
| 36:1:2544:U:H2'   | 36:1:2545:C:C6     | 2.45                     | 0.51              |
| 39:L2:204:MET:HE3 | 39:L2:209:HIS:HB2  | 1.90                     | 0.51              |
| 40:L3:92:TYR:HB2  | 40:L3:157:VAL:HG22 | 1.92                     | 0.51              |
| 67:O1:17:HIS:HB2  | 67:O1:69:TYR:HB3   | 1.92                     | 0.51              |
| 79:Q3:13:LYS:HE3  | 79:Q3:14:TYR:CZ    | 2.45                     | 0.51              |
| 1:6:78:A:C8       | 8:s6:154:ARG:HD3   | 2.45                     | 0.51              |
| 1:6:381:C:OP1     | 6:s4:10:LYS:HD3    | 2.10                     | 0.51              |
| 1:6:595:G:H2'     | 1:6:596:C:C6       | 2.45                     | 0.51              |
| 1:6:794:U:H4'     | 1:6:795:U:OP2      | 2.10                     | 0.51              |
| 1:6:1064:G:H2'    | 1:6:1065:A:C8      | 2.46                     | 0.51              |
| 1:6:1163:A:O3'    | 7:s5:166:ARG:NH2   | 2.43                     | 0.51              |
| 1:6:1366:U:O2'    | 21:c9:7:ARG:HD2    | 2.10                     | 0.51              |
| 3:s1:126:THR:CG2  | 3:s1:136:ARG:HE    | 2.22                     | 0.51              |
| 5:s3:183:GLY:O    | 5:s3:184:ILE:HD13  | 2.10                     | 0.51              |
| 11:s9:149:ARG:HG2 | 11:s9:149:ARG:HH11 | 1.75                     | 0.51              |
| 36:5:2927:C:H2'   | 36:5:2928:C:C6     | 2.45                     | 0.51              |
| 42:l5:226:TYR:CE1 | 42:l5:236:LEU:HD11 | 2.45                     | 0.51              |
| 43:l6:176:PHE:HA  | 50:m4:114:ASP:HB2  | 1.93                     | 0.51              |
| 46:l9:37:ASN:OD1  | 46:l9:39:LYS:HB2   | 2.10                     | 0.51              |
| 54:m8:96:PHE:CG   | 54:m8:97:PRO:HD2   | 2.45                     | 0.51              |
| 72:o6:33:ALA:O    | 72:o6:34:SER:HB3   | 2.08                     | 0.51              |
| 75:o9:15:LYS:O    | 75:o9:19:GLN:HG2   | 2.10                     | 0.51              |
| 1:2:1248:C:H2'    | 1:2:1249:U:C6      | 2.44                     | 0.51              |
| 11:S9:91:LYS:O    | 11:S9:92:LYS:HG2   | 2.10                     | 0.51              |
| 17:C5:15:HIS:O    | 17:C5:21:ASP:HA    | 2.09                     | 0.51              |
| 36:1:428:A:H2'    | 36:1:429:U:C6      | 2.45                     | 0.51              |
| 36:1:715:A:H5''   | 64:N8:114:GLY:O    | 2.10                     | 0.51              |
| 36:1:1348:U:O2    | 36:1:1349:G:N2     | 2.43                     | 0.51              |
| 36:1:2118:C:H2'   | 36:1:2119:A:O4'    | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:2355:G:H4'    | 53:M7:139:TYR:CE2  | 2.45                     | 0.51              |
| 39:L2:227:ARG:HG2  | 39:L2:239:ALA:HB2  | 1.91                     | 0.51              |
| 48:M1:82:ARG:HG2   | 48:M1:112:LEU:HB2  | 1.91                     | 0.51              |
| 1:6:558:U:O2       | 1:6:558:U:H2'      | 2.10                     | 0.51              |
| 1:6:1558:U:H3      | 17:c5:122:THR:CG2  | 2.24                     | 0.51              |
| 4:s2:40:LYS:HG3    | 4:s2:247:ALA:HB1   | 1.92                     | 0.51              |
| 6:s4:192:ILE:HG13  | 6:s4:243:GLY:HA3   | 1.93                     | 0.51              |
| 12:c0:24:LYS:HB2   | 12:c0:63:TYR:CE1   | 2.46                     | 0.51              |
| 36:5:726:G:C5'     | 36:5:726:G:H8      | 2.22                     | 0.51              |
| 36:5:2244:A:H5''   | 39:l2:243:THR:OG1  | 2.10                     | 0.51              |
| 86:5:4066:OHX:N3   | 86:5:4141:OHX:N4   | 2.57                     | 0.51              |
| 37:7:28:C:OP1      | 48:m1:137:ARG:HD3  | 2.11                     | 0.51              |
| 51:m5:135:VAL:HG13 | 51:m5:142:ILE:HG12 | 1.92                     | 0.51              |
| 61:n5:132:ALA:O    | 61:n5:135:ILE:HG22 | 2.10                     | 0.51              |
| 79:q3:27:LYS:O     | 79:q3:31:ILE:HG13  | 2.10                     | 0.51              |
| 82:p0:7:LYS:NZ     | 82:p0:10:GLU:OE1   | 2.36                     | 0.51              |
| 1:2:584:C:H1'      | 32:E0:18:THR:HG21  | 1.91                     | 0.51              |
| 1:2:702:G:C6       | 1:2:737:A:N6       | 2.79                     | 0.51              |
| 2:S0:41:ARG:HD2    | 2:S0:42:PRO:O      | 2.11                     | 0.51              |
| 2:S0:136:ALA:HB1   | 2:S0:141:ILE:HB    | 1.92                     | 0.51              |
| 8:S6:142:ARG:O     | 8:S6:146:GLY:N     | 2.43                     | 0.51              |
| 12:C0:16:PHE:O     | 12:C0:88:PRO:HA    | 2.11                     | 0.51              |
| 26:D4:124:ARG:O    | 26:D4:127:LYS:HG3  | 2.10                     | 0.51              |
| 36:1:409:A:OP2     | 86:1:4060:OHX:N5   | 2.43                     | 0.51              |
| 36:1:781:G:OP1     | 54:M8:151:ARG:HD2  | 2.11                     | 0.51              |
| 36:1:3279:A:N6     | 36:1:3280:U:O4     | 2.43                     | 0.51              |
| 86:1:3976:OHX:N6   | 86:1:4159:OHX:N2   | 2.58                     | 0.51              |
| 41:L4:154:THR:O    | 41:L4:157:GLU:HG3  | 2.09                     | 0.51              |
| 66:O0:17:VAL:HG11  | 66:O0:92:ILE:HD12  | 1.92                     | 0.51              |
| 1:6:1227:A:H4'     | 1:6:1228:G:H5'     | 1.92                     | 0.51              |
| 1:6:1654:G:OP1     | 77:q1:21:ARG:HD2   | 2.11                     | 0.51              |
| 5:s3:107:PHE:O     | 5:s3:111:ASN:HB2   | 2.10                     | 0.51              |
| 5:s3:170:THR:HG22  | 5:s3:187:LYS:HA    | 1.92                     | 0.51              |
| 14:c2:125:ASN:CG   | 35:sM:168:GLU:H    | 2.19                     | 0.51              |
| 36:5:1232:C:C5     | 36:5:1261:G:H2'    | 2.45                     | 0.51              |
| 36:5:2201:G:N2     | 39:l2:224:THR:HG21 | 2.23                     | 0.51              |
| 36:5:2425:G:H2'    | 36:5:2426:U:O4'    | 2.11                     | 0.51              |
| 36:5:2530:G:H2'    | 36:5:2531:C:H5'    | 1.92                     | 0.51              |
| 37:7:7:G:OP1       | 42:l5:33:ARG:HD2   | 2.11                     | 0.51              |
| 41:l4:145:ILE:O    | 41:l4:145:ILE:HG12 | 2.09                     | 0.51              |
| 52:m6:65:ASN:O     | 52:m6:68:ARG:HG2   | 2.11                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:647:G:H22      | 1:2:687:G:N2       | 2.07                     | 0.51              |
| 10:S8:136:SER:HB3  | 10:S8:139:ALA:HB3  | 1.92                     | 0.51              |
| 21:C9:57:ARG:HH21  | 21:C9:80:TYR:HB3   | 1.73                     | 0.51              |
| 24:D2:36:LYS:O     | 24:D2:40:VAL:HG23  | 2.10                     | 0.51              |
| 36:1:520:U:O4      | 41:L4:349:THR:HG23 | 2.11                     | 0.51              |
| 36:1:1580:A:H4'    | 36:1:1581:C:O5'    | 2.11                     | 0.51              |
| 36:1:2656:A:H4'    | 78:Q2:98:LYS:HD2   | 1.92                     | 0.51              |
| 36:1:3041:U:OP1    | 59:N3:12:ARG:NH1   | 2.36                     | 0.51              |
| 86:1:4032:OHX:N4   | 86:1:4149:OHX:N3   | 2.57                     | 0.51              |
| 37:3:22:A:H1'      | 42:L5:272:TYR:CZ   | 2.45                     | 0.51              |
| 86:3:218:OHX:N2    | 86:3:223:OHX:N1    | 2.58                     | 0.51              |
| 41:L4:118:LYS:O    | 41:L4:122:THR:HG23 | 2.10                     | 0.51              |
| 46:L9:84:LYS:CE    | 46:L9:191:LEU:HD13 | 2.41                     | 0.51              |
| 73:O7:14:LYS:HE2   | 75:O9:51:ILE:HG13  | 1.93                     | 0.51              |
| 1:6:594:A:OP2      | 11:s9:37:LYS:HE2   | 2.10                     | 0.51              |
| 1:6:1321:A:OP2     | 2:s0:101:ARG:NH2   | 2.36                     | 0.51              |
| 16:c4:131:GLY:O    | 16:c4:133:ARG:N    | 2.42                     | 0.51              |
| 17:c5:18:ARG:NH1   | 20:c8:90:ASN:O     | 2.44                     | 0.51              |
| 21:c9:100:ILE:O    | 21:c9:104:VAL:HG23 | 2.09                     | 0.51              |
| 33:e1:121:CYS:HB3  | 33:e1:130:VAL:HG11 | 1.93                     | 0.51              |
| 34:sR:198:ASN:O    | 34:sR:215:GLY:HA3  | 2.10                     | 0.51              |
| 34:sR:276:PRO:HB2  | 34:sR:278:PHE:CE1  | 2.46                     | 0.51              |
| 36:5:742:G:N7      | 86:5:4003:OHX:N4   | 2.58                     | 0.51              |
| 36:5:1667:A:H2'    | 36:5:1668:G:C8     | 2.45                     | 0.51              |
| 36:5:3186:A:N3     | 46:l9:44:THR:HG22  | 2.26                     | 0.51              |
| 86:5:3924:OHX:N5   | 38:8:17:A:OP1      | 2.43                     | 0.51              |
| 86:5:3978:OHX:N6   | 86:5:4196:OHX:N5   | 2.59                     | 0.51              |
| 42:l5:152:ARG:HG3  | 42:l5:152:ARG:NH1  | 2.26                     | 0.51              |
| 72:o6:33:ALA:HB1   | 72:o6:38:LYS:HD2   | 1.93                     | 0.51              |
| 1:2:1387:G:OP1     | 19:C7:32:LYS:NZ    | 2.34                     | 0.51              |
| 1:2:1766:A:H5''    | 86:2:2093:OHX:N6   | 2.26                     | 0.51              |
| 6:S4:240:LYS:H     | 6:S4:240:LYS:HE2   | 1.75                     | 0.51              |
| 28:D6:38:ARG:HH21  | 28:D6:83:ILE:HG13  | 1.76                     | 0.51              |
| 36:1:2676:A:N1     | 48:M1:22:SER:OG    | 2.43                     | 0.51              |
| 86:1:4084:OHX:N6   | 86:1:4153:OHX:N5   | 2.58                     | 0.51              |
| 42:L5:107:ARG:HH21 | 42:L5:110:LEU:HD23 | 1.76                     | 0.51              |
| 61:N5:132:ALA:O    | 61:N5:135:ILE:HG22 | 2.11                     | 0.51              |
| 1:6:93:A:O4'       | 6:s4:3:ARG:NH1     | 2.43                     | 0.51              |
| 1:6:600:U:OP2      | 25:d3:108:GLY:HA2  | 2.10                     | 0.51              |
| 1:6:1471:A:H5'     | 7:s5:184:PHE:CE2   | 2.45                     | 0.51              |
| 2:s0:163:ASN:C     | 2:s0:165:ARG:H     | 2.17                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:s5:43:PHE:HB3   | 7:s5:46:TRP:CD1    | 2.46                     | 0.51              |
| 36:5:715:A:C8     | 64:n8:115:LYS:HG3  | 2.42                     | 0.51              |
| 36:5:1196:C:OP1   | 86:5:4235:OHX:N6   | 2.44                     | 0.51              |
| 36:5:1233:G:H5'   | 82:p0:36:GLN:OE1   | 2.10                     | 0.51              |
| 36:5:1328:C:H2'   | 36:5:1329:U:C6     | 2.45                     | 0.51              |
| 54:m8:76:ALA:HA   | 54:m8:79:LYS:HD2   | 1.93                     | 0.51              |
| 65:n9:21:ILE:HG22 | 65:n9:22:LYS:N     | 2.25                     | 0.51              |
| 66:o0:99:ASP:OD2  | 66:o0:99:ASP:N     | 2.42                     | 0.51              |
| 82:p0:81:LYS:HD3  | 82:p0:82:GLY:H     | 1.76                     | 0.51              |
| 1:2:1274:C:C5     | 35:SM:96:ARG:HG3   | 2.45                     | 0.51              |
| 12:C0:15:LEU:HD13 | 12:C0:21:VAL:HG23  | 1.93                     | 0.51              |
| 26:D4:29:HIS:CE1  | 26:D4:34:ASN:H     | 2.29                     | 0.51              |
| 36:1:112:U:O2'    | 36:1:113:C:OP2     | 2.26                     | 0.51              |
| 36:1:191:U:H2'    | 36:1:192:C:C6      | 2.45                     | 0.51              |
| 36:1:863:C:H2'    | 36:1:864:G:O4'     | 2.09                     | 0.51              |
| 36:1:3002:C:O2'   | 40:L3:180:GLU:OE2  | 2.21                     | 0.51              |
| 69:O3:49:ILE:HG23 | 69:O3:100:ILE:HG13 | 1.93                     | 0.51              |
| 71:O5:115:LYS:HB2 | 71:O5:115:LYS:NZ   | 2.26                     | 0.51              |
| 4:s2:178:ILE:HB   | 4:s2:185:LYS:HG2   | 1.93                     | 0.51              |
| 7:s5:162:VAL:HG22 | 7:s5:167:ARG:HG2   | 1.92                     | 0.51              |
| 12:c0:46:LEU:HA   | 12:c0:49:LEU:HB2   | 1.93                     | 0.51              |
| 36:5:998:A:O2'    | 36:5:999:G:H5'     | 2.11                     | 0.51              |
| 36:5:2428:U:O4    | 86:5:4214:OHX:N5   | 2.43                     | 0.51              |
| 36:5:2939:G:OP2   | 40:l3:2:SER:O      | 2.27                     | 0.51              |
| 38:8:78:G:H2'     | 38:8:79:A:O4'      | 2.09                     | 0.51              |
| 81:m2:52:UNK:C    | 81:m2:54:UNK:H     | 2.23                     | 0.51              |
| 1:2:16:G:H2'      | 1:2:17:C:C6        | 2.45                     | 0.51              |
| 1:2:505:A:H2'     | 1:2:505:A:N3       | 2.24                     | 0.51              |
| 3:S1:180:THR:HG22 | 3:S1:181:LEU:H     | 1.75                     | 0.51              |
| 3:S1:183:GLN:O    | 3:S1:187:LYS:N     | 2.44                     | 0.51              |
| 9:S7:58:LEU:N     | 9:S7:89:HIS:O      | 2.40                     | 0.51              |
| 11:S9:89:ASP:HB2  | 11:S9:90:LYS:HD3   | 1.93                     | 0.51              |
| 17:C5:19:GLY:N    | 20:C8:93:THR:O     | 2.44                     | 0.51              |
| 26:D4:112:LYS:O   | 26:D4:116:LYS:HG3  | 2.11                     | 0.51              |
| 33:E1:117:LEU:HB3 | 33:E1:118:ARG:HH11 | 1.74                     | 0.51              |
| 36:1:904:A:OP2    | 73:O7:30:GLN:NE2   | 2.38                     | 0.51              |
| 36:1:3112:G:O2'   | 46:L9:70:THR:HB    | 2.11                     | 0.51              |
| 37:3:79:A:C2      | 37:3:102:A:C4      | 2.99                     | 0.51              |
| 40:L3:232:ARG:HG2 | 40:L3:233:TRP:CD1  | 2.46                     | 0.51              |
| 44:L7:92:ILE:HG13 | 54:M8:4:ASP:HB2    | 1.91                     | 0.51              |
| 49:M3:166:ALA:N   | 64:N8:135:GLU:OE1  | 2.20                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:N7:23:VAL:HB    | 63:N7:43:VAL:HB    | 1.92                     | 0.51              |
| 64:N8:77:LYS:O     | 64:N8:79:TRP:N     | 2.44                     | 0.51              |
| 69:O3:51:TYR:HD2   | 69:O3:67:MET:HE3   | 1.75                     | 0.51              |
| 1:6:197:A:H2'      | 1:6:198:A:C8       | 2.46                     | 0.51              |
| 1:6:1268:G:H1'     | 1:6:1448:G:H5''    | 1.93                     | 0.51              |
| 6:s4:11:ARG:HB2    | 6:s4:27:TYR:C      | 2.35                     | 0.51              |
| 7:s5:59:VAL:C      | 7:s5:61:TYR:H      | 2.19                     | 0.51              |
| 20:c8:140:THR:HA   | 20:c8:143:ARG:HH11 | 1.74                     | 0.51              |
| 26:d4:121:THR:CG2  | 26:d4:123:LYS:HB2  | 2.41                     | 0.51              |
| 36:5:549:U:H2'     | 36:5:550:A:C8      | 2.45                     | 0.51              |
| 36:5:806:A:H5''    | 36:5:936:A:H61     | 1.75                     | 0.51              |
| 36:5:2683:U:H2'    | 36:5:2684:C:H6     | 1.76                     | 0.51              |
| 36:5:2799:A:H5''   | 36:5:2800:G:O5'    | 2.10                     | 0.51              |
| 38:8:59:A:H5''     | 38:8:61:A:C8       | 2.45                     | 0.51              |
| 61:n5:105:VAL:HG13 | 61:n5:130:TYR:CG   | 2.46                     | 0.51              |
| 1:2:1180:C:O2'     | 17:C5:128:HIS:ND1  | 2.42                     | 0.51              |
| 1:2:1528:U:OP1     | 7:S5:109:LYS:HG2   | 2.11                     | 0.51              |
| 1:2:1590:G:OP1     | 21:C9:91:TYR:HB2   | 2.11                     | 0.51              |
| 12:C0:11:ILE:HD12  | 12:C0:42:VAL:HA    | 1.91                     | 0.51              |
| 16:C4:17:ALA:HB3   | 16:C4:81:VAL:HA    | 1.91                     | 0.51              |
| 28:D6:60:PRO:C     | 28:D6:62:TYR:H     | 2.18                     | 0.51              |
| 34:SR:42:LEU:HB2   | 34:SR:61:PHE:HB2   | 1.93                     | 0.51              |
| 36:1:1555:U:H5     | 36:1:1559:A:H61    | 1.58                     | 0.51              |
| 42:L5:106:ALA:O    | 42:L5:110:LEU:HB2  | 2.11                     | 0.51              |
| 45:L8:91:PHE:O     | 45:L8:95:ASN:HB2   | 2.11                     | 0.51              |
| 55:M9:28:GLU:O     | 55:M9:32:ILE:HG13  | 2.11                     | 0.51              |
| 57:N1:56:PHE:CZ    | 57:N1:78:LYS:HD3   | 2.45                     | 0.51              |
| 64:N8:90:TYR:CG    | 64:N8:100:PRO:HG3  | 2.46                     | 0.51              |
| 1:6:699:U:O4       | 86:6:2074:OHX:N1   | 2.43                     | 0.51              |
| 1:6:846:G:H2'      | 1:6:847:A:C8       | 2.45                     | 0.51              |
| 13:c1:33:ARG:NH1   | 13:c1:53:TYR:O     | 2.44                     | 0.51              |
| 14:c2:72:ILE:O     | 14:c2:76:GLU:HB2   | 2.10                     | 0.51              |
| 18:c6:78:VAL:O     | 18:c6:81:ILE:HG12  | 2.11                     | 0.51              |
| 27:d5:38:HIS:ND1   | 27:d5:70:LYS:HG2   | 2.26                     | 0.51              |
| 36:5:73:C:C2       | 49:m3:59:ARG:HD3   | 2.46                     | 0.51              |
| 36:5:210:U:O2      | 41:l4:217:LYS:HE2  | 2.11                     | 0.51              |
| 36:5:609:G:OP2     | 41:l4:315:LYS:NZ   | 2.26                     | 0.51              |
| 36:5:1629:U:O4     | 63:n7:111:LYS:HE2  | 2.11                     | 0.51              |
| 36:5:2427:U:H2'    | 36:5:2428:U:C6     | 2.46                     | 0.51              |
| 86:5:3978:OHX:N4   | 86:5:4196:OHX:N3   | 2.59                     | 0.51              |
| 39:l2:116:VAL:HG23 | 39:l2:117:GLU:O    | 2.11                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:n2:89:LEU:HB3  | 58:n2:93:ILE:HD12  | 1.92                     | 0.51              |
| 62:n6:83:ASP:O    | 62:n6:84:LYS:HB2   | 2.11                     | 0.51              |
| 67:o1:75:ILE:HG12 | 67:o1:93:VAL:HG13  | 1.91                     | 0.51              |
| 70:o4:74:ARG:HG2  | 70:o4:75:ALA:N     | 2.26                     | 0.51              |
| 74:o8:39:ARG:HH12 | 74:o8:63:LYS:HE2   | 1.74                     | 0.51              |
| 82:p0:3:GLY:O     | 82:p0:6:GLU:HB3    | 2.11                     | 0.51              |
| 82:p0:69:ASP:OD1  | 82:p0:69:ASP:N     | 2.43                     | 0.51              |
| 1:2:114:C:H5'     | 1:2:114:C:H6       | 1.76                     | 0.51              |
| 1:2:611:U:OP1     | 25:D3:19:ARG:NH2   | 2.44                     | 0.51              |
| 1:2:1662:G:O2'    | 1:2:1663:G:H5'     | 2.11                     | 0.51              |
| 6:S4:36:HIS:ND1   | 6:S4:85:GLY:HA3    | 2.26                     | 0.51              |
| 6:S4:185:GLY:H    | 6:S4:189:LEU:HD13  | 1.76                     | 0.51              |
| 9:S7:30:SER:O     | 9:S7:34:LEU:HB2    | 2.11                     | 0.51              |
| 12:C0:14:TYR:HE2  | 12:C0:21:VAL:HG22  | 1.76                     | 0.51              |
| 36:1:2208:A:N1    | 86:1:4047:OHX:N4   | 2.59                     | 0.51              |
| 36:1:2333:C:H2'   | 36:1:2334:U:O4'    | 2.11                     | 0.51              |
| 40:L3:244:ARG:NH1 | 40:L3:244:ARG:HG2  | 2.26                     | 0.51              |
| 44:L7:89:ILE:HG13 | 44:L7:214:TRP:CH2  | 2.46                     | 0.51              |
| 47:M0:206:LEU:O   | 47:M0:210:ILE:HG13 | 2.11                     | 0.51              |
| 52:M6:65:ASN:O    | 52:M6:68:ARG:HG2   | 2.10                     | 0.51              |
| 55:M9:23:TRP:HB2  | 55:M9:53:LYS:HD2   | 1.93                     | 0.51              |
| 62:N6:79:ALA:HB1  | 62:N6:98:ASN:HB3   | 1.92                     | 0.51              |
| 1:6:291:G:H2'     | 1:6:292:U:C6       | 2.46                     | 0.51              |
| 1:6:648:G:C2      | 1:6:687:G:C2       | 2.98                     | 0.51              |
| 1:6:944:A:OP2     | 28:d6:19:LYS:NZ    | 2.43                     | 0.51              |
| 1:6:1350:U:H2'    | 1:6:1351:G:H8      | 1.74                     | 0.51              |
| 11:s9:39:LYS:HB3  | 11:s9:43:TYR:CZ    | 2.45                     | 0.51              |
| 19:c7:44:LYS:HG3  | 19:c7:47:ARG:HH12  | 1.75                     | 0.51              |
| 22:d0:100:VAL:O   | 22:d0:104:THR:HG23 | 2.11                     | 0.51              |
| 36:5:2356:A:OP1   | 53:m7:138:LYS:NZ   | 2.41                     | 0.51              |
| 36:5:3341:U:H5''  | 36:5:3342:A:OP2    | 2.10                     | 0.51              |
| 86:5:4054:OHX:N3  | 86:5:4108:OHX:N5   | 2.59                     | 0.51              |
| 86:5:4094:OHX:N1  | 86:5:4234:OHX:N2   | 2.59                     | 0.51              |
| 48:m1:59:ILE:HD12 | 48:m1:65:ILE:HD11  | 1.93                     | 0.51              |
| 50:m4:47:ASP:OD1  | 50:m4:55:ARG:HB2   | 2.10                     | 0.51              |
| 50:m4:49:PRO:HG3  | 50:m4:78:THR:HG23  | 1.93                     | 0.51              |
| 52:m6:143:THR:OG1 | 52:m6:150:GLU:OE2  | 2.24                     | 0.51              |
| 66:o0:61:MET:HG3  | 66:o0:62:LEU:N     | 2.26                     | 0.51              |
| 71:o5:86:ARG:O    | 71:o5:90:ARG:HG2   | 2.11                     | 0.51              |
| 1:2:793:A:H5''    | 1:2:794:U:C6       | 2.46                     | 0.51              |
| 7:S5:29:ILE:HG21  | 18:C6:57:LEU:HD11  | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:C1:22:ASN:ND2   | 13:C1:25:VAL:HG23  | 2.26                     | 0.51              |
| 19:C7:37:GLU:HG3   | 34:SR:150:TRP:HE1  | 1.75                     | 0.51              |
| 22:D0:105:GLN:HG3  | 22:D0:106:ILE:N    | 2.26                     | 0.51              |
| 33:E1:130:VAL:HG11 | 33:E1:143:LYS:HG2  | 1.92                     | 0.51              |
| 36:1:522:A:OP1     | 86:1:3948:OHX:N5   | 2.43                     | 0.51              |
| 36:1:1482:A:H4'    | 36:1:1483:G:OP2    | 2.10                     | 0.51              |
| 36:1:2366:C:H5'    | 40:L3:259:HIS:NE2  | 2.26                     | 0.51              |
| 36:1:2636:A:H5''   | 36:1:2637:A:H5'    | 1.93                     | 0.51              |
| 36:1:3217:C:O2     | 36:1:3217:C:H2'    | 2.11                     | 0.51              |
| 41:L4:140:HIS:HA   | 41:L4:177:ASP:OD1  | 2.11                     | 0.51              |
| 52:M6:110:PRO:HA   | 52:M6:113:ASP:OD2  | 2.10                     | 0.51              |
| 1:6:336:G:OP2      | 86:6:2155:OHX:N4   | 2.44                     | 0.51              |
| 1:6:1482:C:OP2     | 1:6:1521:G:N1      | 2.42                     | 0.51              |
| 6:s4:132:GLY:N     | 6:s4:136:VAL:O     | 2.43                     | 0.51              |
| 17:c5:33:PHE:O     | 17:c5:36:LEU:HD22  | 2.10                     | 0.51              |
| 25:d3:70:LYS:HB3   | 25:d3:93:LEU:HD22  | 1.92                     | 0.51              |
| 26:d4:50:ALA:HB1   | 26:d4:54:ALA:HB3   | 1.93                     | 0.51              |
| 36:5:135:C:H4'     | 36:5:136:G:OP2     | 2.10                     | 0.51              |
| 36:5:815:G:C6      | 36:5:906:A:C4      | 2.99                     | 0.51              |
| 36:5:1318:A:OP1    | 52:m6:18:ARG:NH2   | 2.44                     | 0.51              |
| 36:5:2195:C:OP2    | 86:5:4204:OHX:N4   | 2.44                     | 0.51              |
| 36:5:2239:G:N7     | 86:5:4190:OHX:N5   | 2.58                     | 0.51              |
| 36:5:2418:G:O6     | 86:5:4247:OHX:N2   | 2.44                     | 0.51              |
| 36:5:2550:U:H5     | 39:l2:40:TYR:O     | 1.93                     | 0.51              |
| 36:5:2935:U:O2     | 36:5:2935:U:H2'    | 2.11                     | 0.51              |
| 36:5:3318:G:OP2    | 86:5:4138:OHX:N5   | 2.44                     | 0.51              |
| 40:l3:313:HIS:O    | 40:l3:333:LYS:HE3  | 2.11                     | 0.51              |
| 42:l5:64:ILE:HD12  | 42:l5:144:VAL:HG21 | 1.93                     | 0.51              |
| 44:l7:110:ARG:NH2  | 54:m8:3:ILE:HD12   | 2.25                     | 0.51              |
| 50:m4:134:ALA:C    | 50:m4:136:ALA:H    | 2.19                     | 0.51              |
| 66:o0:13:LYS:HE3   | 66:o0:103:THR:HG21 | 1.93                     | 0.51              |
| 82:p0:19:LEU:HD22  | 82:p0:73:PHE:CE1   | 2.45                     | 0.51              |
| 1:2:711:U:H1'      | 1:2:712:G:C8       | 2.46                     | 0.50              |
| 1:2:734:A:H4'      | 1:2:735:C:H5'      | 1.93                     | 0.50              |
| 1:2:796:A:OP2      | 86:2:2058:OHX:N6   | 2.44                     | 0.50              |
| 1:2:1291:G:N2      | 1:2:1324:G:N2      | 2.59                     | 0.50              |
| 2:S0:193:GLN:C     | 2:S0:195:TRP:H     | 2.19                     | 0.50              |
| 20:C8:54:LEU:H     | 20:C8:54:LEU:HD22  | 1.77                     | 0.50              |
| 22:D0:80:GLU:HG3   | 31:D9:54:LYS:NZ    | 2.26                     | 0.50              |
| 24:D2:104:LEU:HB2  | 24:D2:124:LYS:O    | 2.11                     | 0.50              |
| 34:SR:70:ASP:OD1   | 34:SR:71:CYS:N     | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:SM:84:LYS:HG2  | 35:SM:86:ASN:H     | 1.76                     | 0.50              |
| 36:1:900:G:H1'    | 36:1:1589:A:H61    | 1.76                     | 0.50              |
| 36:1:3269:U:H4'   | 36:1:3270:U:O5'    | 2.12                     | 0.50              |
| 36:1:3330:A:H5''  | 36:1:3330:A:H8     | 1.76                     | 0.50              |
| 40:L3:261:MET:HE2 | 52:M6:64:PHE:HA    | 1.93                     | 0.50              |
| 49:M3:109:PHE:O   | 49:M3:113:VAL:HG23 | 2.10                     | 0.50              |
| 54:M8:41:ASP:C    | 54:M8:41:ASP:OD1   | 2.54                     | 0.50              |
| 63:N7:21:LYS:HE3  | 63:N7:47:GLU:O     | 2.10                     | 0.50              |
| 1:6:1081:A:H1'    | 1:6:1082:C:C5      | 2.46                     | 0.50              |
| 2:s0:184:LEU:O    | 2:s0:186:GLY:N     | 2.44                     | 0.50              |
| 3:s1:175:GLU:HG2  | 3:s1:193:ILE:CD1   | 2.41                     | 0.50              |
| 7:s5:129:PRO:O    | 7:s5:132:VAL:HB    | 2.11                     | 0.50              |
| 18:c6:37:THR:O    | 18:c6:45:ARG:NH1   | 2.44                     | 0.50              |
| 20:c8:86:LEU:HG   | 20:c8:99:HIS:HB2   | 1.93                     | 0.50              |
| 28:d6:34:LYS:O    | 28:d6:35:ALA:HB3   | 2.11                     | 0.50              |
| 36:5:94:G:H2'     | 36:5:95:A:C8       | 2.46                     | 0.50              |
| 36:5:269:G:H5''   | 51:m5:14:LYS:HE2   | 1.93                     | 0.50              |
| 36:5:853:G:N7     | 79:q3:2:ALA:HB2    | 2.26                     | 0.50              |
| 36:5:1157:G:H2'   | 36:5:1158:A:O4'    | 2.11                     | 0.50              |
| 36:5:3316:A:O2'   | 86:5:4249:OHX:N3   | 2.45                     | 0.50              |
| 46:l9:143:GLU:O   | 46:l9:144:ILE:HG22 | 2.10                     | 0.50              |
| 48:m1:8:PRO:CD    | 48:m1:9:MET:H      | 2.24                     | 0.50              |
| 81:m2:48:UNK:O    | 81:m2:51:UNK:N     | 2.44                     | 0.50              |
| 49:m3:129:ASN:CG  | 49:m3:130:GLY:H    | 2.18                     | 0.50              |
| 51:m5:14:LYS:HA   | 51:m5:19:LEU:HD23  | 1.92                     | 0.50              |
| 78:q2:71:ARG:HH11 | 78:q2:71:ARG:CG    | 2.24                     | 0.50              |
| 84:p2:16:UNK:O    | 84:p2:18:UNK:N     | 2.43                     | 0.50              |
| 1:2:337:G:H3'     | 13:C1:133:LYS:HB2  | 1.93                     | 0.50              |
| 1:2:652:G:H1      | 1:2:682:C:H42      | 1.58                     | 0.50              |
| 1:2:702:G:O6      | 1:2:737:A:N6       | 2.44                     | 0.50              |
| 4:S2:90:THR:HG23  | 4:S2:92:ALA:H      | 1.76                     | 0.50              |
| 28:D6:10:ARG:NH1  | 28:D6:36:ILE:HA    | 2.27                     | 0.50              |
| 36:1:670:C:P      | 54:M8:147:ARG:NH2  | 2.84                     | 0.50              |
| 36:1:1812:G:O2'   | 36:1:1818:U:H4'    | 2.11                     | 0.50              |
| 36:1:2443:A:N6    | 36:1:2504:U:C4     | 2.79                     | 0.50              |
| 86:1:3964:OHX:N5  | 86:1:4143:OHX:N6   | 2.59                     | 0.50              |
| 86:1:3968:OHX:N3  | 86:1:4076:OHX:N4   | 2.58                     | 0.50              |
| 46:L9:163:GLN:HA  | 46:L9:166:ARG:HD2  | 1.93                     | 0.50              |
| 56:N0:155:ARG:HD3 | 56:N0:172:TYR:CD2  | 2.46                     | 0.50              |
| 57:N1:71:SER:HB3  | 57:N1:91:LEU:O     | 2.10                     | 0.50              |
| 61:N5:115:ARG:NH1 | 61:N5:119:THR:OG1  | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:O0:98:SER:OG    | 66:O0:99:ASP:N     | 2.43                     | 0.50              |
| 1:6:931:C:OP1      | 28:d6:70:LYS:HE3   | 2.11                     | 0.50              |
| 1:6:1657:U:HO2'    | 1:6:1658:G:P       | 2.29                     | 0.50              |
| 1:6:1750:A:OP1     | 77:q1:16:LYS:NZ    | 2.43                     | 0.50              |
| 4:s2:97:ARG:HB2    | 4:s2:118:ALA:O     | 2.11                     | 0.50              |
| 7:s5:92:ARG:NH2    | 7:s5:169:ASN:OD1   | 2.44                     | 0.50              |
| 26:d4:57:VAL:HB    | 26:d4:60:PHE:HE2   | 1.76                     | 0.50              |
| 36:5:947:G:H5'     | 68:o2:55:ILE:HB    | 1.92                     | 0.50              |
| 38:8:145:U:H2'     | 38:8:146:U:C6      | 2.46                     | 0.50              |
| 40:l3:46:PHE:CE2   | 40:l3:205:VAL:HG13 | 2.46                     | 0.50              |
| 53:m7:79:THR:HG22  | 53:m7:80:LYS:HG3   | 1.93                     | 0.50              |
| 57:n1:12:ARG:HD3   | 57:n1:13:TYR:CE1   | 2.46                     | 0.50              |
| 63:n7:36:HIS:CD2   | 63:n7:74:VAL:HG11  | 2.45                     | 0.50              |
| 75:o9:50:ASN:O     | 75:o9:51:ILE:HB    | 2.12                     | 0.50              |
| 1:2:538:A:H8       | 1:2:543:C:N4       | 2.09                     | 0.50              |
| 1:2:1031:U:H4'     | 1:2:1032:G:OP2     | 2.10                     | 0.50              |
| 3:S1:62:LYS:O      | 3:S1:64:ARG:N      | 2.33                     | 0.50              |
| 33:E1:98:VAL:HG22  | 33:E1:99:LYS:H     | 1.76                     | 0.50              |
| 36:1:170:G:C4      | 36:1:250:U:O2      | 2.65                     | 0.50              |
| 36:1:1567:U:H5     | 36:1:1568:U:C2     | 2.28                     | 0.50              |
| 36:1:2396:G:OP1    | 36:1:2397:A:H4'    | 2.11                     | 0.50              |
| 36:1:2747:A:H5'    | 42:L5:175:HIS:HA   | 1.93                     | 0.50              |
| 40:L3:56:ILE:HD11  | 40:L3:359:ILE:HG12 | 1.91                     | 0.50              |
| 40:L3:299:ASP:OD1  | 40:L3:301:THR:HG23 | 2.12                     | 0.50              |
| 50:M4:128:ARG:HG2  | 50:M4:132:LYS:HG3  | 1.94                     | 0.50              |
| 53:M7:182:ILE:HG22 | 53:M7:183:ALA:N    | 2.25                     | 0.50              |
| 3:s1:38:PHE:CD1    | 3:s1:73:LEU:HG     | 2.46                     | 0.50              |
| 12:c0:34:GLU:O     | 12:c0:35:ILE:HB    | 2.11                     | 0.50              |
| 14:c2:66:VAL:HG11  | 14:c2:72:ILE:HG13  | 1.93                     | 0.50              |
| 16:c4:20:TYR:HB3   | 16:c4:27:PHE:HB2   | 1.92                     | 0.50              |
| 19:c7:26:LEU:HD23  | 19:c7:58:MET:HB3   | 1.93                     | 0.50              |
| 26:d4:122:GLY:O    | 26:d4:125:LEU:N    | 2.44                     | 0.50              |
| 36:5:114:A:N1      | 36:5:266:A:O2'     | 2.41                     | 0.50              |
| 36:5:221:A:N6      | 62:n6:103:LYS:HZ1  | 2.09                     | 0.50              |
| 36:5:1232:C:H2'    | 36:5:1233:G:H8     | 1.76                     | 0.50              |
| 36:5:2557:A:OP1    | 39:l2:69:TYR:OH    | 2.27                     | 0.50              |
| 86:5:4000:OHX:N2   | 86:5:4190:OHX:N1   | 2.60                     | 0.50              |
| 40:l3:366:GLY:O    | 40:l3:368:GLY:N    | 2.44                     | 0.50              |
| 41:l4:271:LYS:HB2  | 41:l4:274:TYR:CB   | 2.41                     | 0.50              |
| 41:l4:286:VAL:HG11 | 54:m8:31:LYS:HD2   | 1.92                     | 0.50              |
| 46:l9:109:ALA:O    | 46:l9:110:LYS:HB2  | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:m8:178:ARG:HD2  | 64:n8:50:PRO:HB2   | 1.92                     | 0.50              |
| 61:n5:105:VAL:HG13 | 61:n5:130:TYR:CD2  | 2.46                     | 0.50              |
| 79:q3:74:ALA:O     | 79:q3:78:THR:HG22  | 2.11                     | 0.50              |
| 1:2:260:U:O2'      | 1:2:261:U:OP1      | 2.29                     | 0.50              |
| 1:2:1039:A:H5''    | 23:D1:62:ARG:NH2   | 2.25                     | 0.50              |
| 1:2:1226:A:O2'     | 1:2:1227:A:OP1     | 2.26                     | 0.50              |
| 1:2:1402:G:OP1     | 19:C7:10:LYS:NZ    | 2.44                     | 0.50              |
| 86:2:2076:OHX:N6   | 86:2:2163:OHX:N2   | 2.59                     | 0.50              |
| 2:S0:35:PRO:C      | 2:S0:37:VAL:H      | 2.20                     | 0.50              |
| 7:S5:161:ASP:O     | 30:D8:44:VAL:HA    | 2.11                     | 0.50              |
| 10:S8:182:TYR:OH   | 10:S8:188:GLU:OE1  | 2.15                     | 0.50              |
| 15:C3:105:ASN:C    | 15:C3:107:LYS:H    | 2.20                     | 0.50              |
| 20:C8:42:TYR:HA    | 20:C8:85:PHE:HE1   | 1.76                     | 0.50              |
| 23:D1:1:MET:HG3    | 23:D1:10:GLU:HB3   | 1.93                     | 0.50              |
| 25:D3:132:LEU:O    | 25:D3:135:LEU:N    | 2.44                     | 0.50              |
| 34:SR:113:VAL:O    | 34:SR:155:ARG:NH1  | 2.44                     | 0.50              |
| 36:1:2177:G:OP2    | 39:L2:128:ARG:HD3  | 2.12                     | 0.50              |
| 36:1:2371:G:O6     | 86:1:3875:OHX:N3   | 2.44                     | 0.50              |
| 36:1:2896:A:H5'    | 36:1:2896:A:H8     | 1.76                     | 0.50              |
| 36:1:3374:U:OP1    | 67:O1:17:HIS:ND1   | 2.38                     | 0.50              |
| 40:L3:296:THR:HG21 | 40:L3:357:LYS:O    | 2.11                     | 0.50              |
| 48:M1:16:LYS:HG2   | 48:M1:130:VAL:HG13 | 1.93                     | 0.50              |
| 49:M3:94:GLY:HA3   | 71:O5:116:TYR:OH   | 2.10                     | 0.50              |
| 50:M4:17:VAL:HG12  | 50:M4:72:LEU:HB3   | 1.92                     | 0.50              |
| 74:O8:4:GLU:HG2    | 74:O8:5:ILE:N      | 2.25                     | 0.50              |
| 1:6:326:G:OP1      | 13:c1:57:LYS:NZ    | 2.41                     | 0.50              |
| 1:6:577:G:N1       | 86:6:2159:OHX:N4   | 2.60                     | 0.50              |
| 1:6:1459:C:OP2     | 20:c8:138:THR:OG1  | 2.20                     | 0.50              |
| 1:6:1729:C:O2'     | 10:s8:2:GLY:HA2    | 2.12                     | 0.50              |
| 3:s1:97:LEU:HB3    | 3:s1:232:HIS:CD2   | 2.47                     | 0.50              |
| 5:s3:48:VAL:HB     | 5:s3:86:LEU:HD12   | 1.93                     | 0.50              |
| 7:s5:43:PHE:H      | 7:s5:46:TRP:H      | 1.59                     | 0.50              |
| 8:s6:214:LYS:HB3   | 8:s6:218:GLU:OE1   | 2.11                     | 0.50              |
| 11:s9:119:ALA:O    | 11:s9:124:HIS:ND1  | 2.33                     | 0.50              |
| 13:c1:73:GLY:HA3   | 13:c1:86:ILE:HG23  | 1.94                     | 0.50              |
| 36:5:429:U:H4'     | 69:o3:88:ASN:HB2   | 1.92                     | 0.50              |
| 36:5:622:A:H2'     | 36:5:623:U:O4'     | 2.11                     | 0.50              |
| 36:5:1281:G:H5'    | 82:p0:55:LYS:HG3   | 1.93                     | 0.50              |
| 36:5:1470:U:H2'    | 36:5:1471:U:C6     | 2.46                     | 0.50              |
| 36:5:1654:A:C2'    | 36:5:1655:G:H5''   | 2.37                     | 0.50              |
| 36:5:2180:G:H2'    | 36:5:2181:C:C6     | 2.46                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:l8:116:VAL:O    | 45:l8:118:GLU:N    | 2.45                     | 0.50              |
| 49:m3:76:THR:HG23  | 49:m3:101:ARG:NH1  | 2.27                     | 0.50              |
| 49:m3:191:ALA:O    | 49:m3:194:GLU:HB2  | 2.11                     | 0.50              |
| 57:n1:56:PHE:CZ    | 57:n1:78:LYS:HD3   | 2.46                     | 0.50              |
| 64:n8:47:LYS:HE3   | 64:n8:48:TYR:CZ    | 2.47                     | 0.50              |
| 1:2:105:A:OP1      | 10:S8:18:ARG:NH1   | 2.44                     | 0.50              |
| 1:2:709:C:C4       | 1:2:710:U:H1'      | 2.46                     | 0.50              |
| 1:2:1274:C:H5      | 35:SM:96:ARG:H     | 1.59                     | 0.50              |
| 3:S1:146:GLN:O     | 3:S1:148:ASN:N     | 2.44                     | 0.50              |
| 6:S4:15:PRO:HG2    | 6:S4:18:TRP:CE2    | 2.47                     | 0.50              |
| 8:S6:4:ASN:HA      | 8:S6:15:THR:HG22   | 1.94                     | 0.50              |
| 9:S7:71:HIS:CG     | 9:S7:131:PHE:HZ    | 2.29                     | 0.50              |
| 10:S8:36:THR:HG23  | 10:S8:96:LEU:O     | 2.11                     | 0.50              |
| 14:C2:131:ASP:HB2  | 14:C2:132:GLU:CD   | 2.37                     | 0.50              |
| 36:1:1556:C:O2'    | 36:1:2169:G:N1     | 2.44                     | 0.50              |
| 36:1:2233:A:OP2    | 86:1:4047:OHX:N5   | 2.44                     | 0.50              |
| 39:L2:217:GLN:O    | 39:L2:218:HIS:HB3  | 2.12                     | 0.50              |
| 43:L6:107:ALA:O    | 43:L6:109:GLU:HG2  | 2.12                     | 0.50              |
| 46:L9:109:ALA:HB1  | 46:L9:111:PHE:CD2  | 2.47                     | 0.50              |
| 53:M7:60:PHE:HB3   | 53:M7:64:ASN:HB3   | 1.92                     | 0.50              |
| 62:N6:37:LYS:H     | 62:N6:37:LYS:CE    | 2.25                     | 0.50              |
| 1:6:212:U:OP2      | 86:c1:202:OHX:N1   | 2.45                     | 0.50              |
| 1:6:895:G:O2'      | 16:c4:37:GLU:HA    | 2.11                     | 0.50              |
| 1:6:1698:G:O2'     | 1:6:1699:G:O5'     | 2.27                     | 0.50              |
| 4:s2:237:VAL:O     | 4:s2:238:SER:OG    | 2.28                     | 0.50              |
| 10:s8:196:LEU:HD22 | 10:s8:200:LYS:HD3  | 1.94                     | 0.50              |
| 13:c1:76:VAL:HG12  | 13:c1:85:VAL:O     | 2.10                     | 0.50              |
| 14:c2:60:VAL:HG22  | 14:c2:122:VAL:HG22 | 1.92                     | 0.50              |
| 80:e0:53:LYS:HE2   | 80:e0:55:ARG:HD3   | 1.92                     | 0.50              |
| 36:5:943:U:H3'     | 64:n8:13:GLY:HA2   | 1.92                     | 0.50              |
| 36:5:2395:G:H5''   | 40:l3:255:TRP:CD1  | 2.46                     | 0.50              |
| 36:5:3237:U:H2'    | 36:5:3238:G:O4'    | 2.12                     | 0.50              |
| 86:5:4011:OHX:N3   | 86:5:4198:OHX:N1   | 2.59                     | 0.50              |
| 42:l5:41:LYS:HB2   | 57:n1:68:THR:O     | 2.12                     | 0.50              |
| 48:m1:133:ARG:HD2  | 48:m1:153:LYS:H    | 1.76                     | 0.50              |
| 77:q1:6:ARG:O      | 77:q1:10:THR:HG23  | 2.11                     | 0.50              |
| 82:p0:37:GLN:HE22  | 82:p0:184:GLY:HA2  | 1.76                     | 0.50              |
| 2:S0:179:ARG:HD3   | 2:S0:183:ARG:NH1   | 2.20                     | 0.50              |
| 10:S8:29:LEU:HD23  | 10:S8:29:LEU:C     | 2.37                     | 0.50              |
| 19:C7:71:PHE:HD1   | 19:C7:73:LEU:HB3   | 1.76                     | 0.50              |
| 30:D8:13:ILE:HD13  | 30:D8:31:GLU:HB2   | 1.94                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:242:C:HO2'    | 36:1:243:G:H8      | 1.59                     | 0.50              |
| 36:1:1547:G:P      | 51:M5:105:ARG:HH11 | 2.34                     | 0.50              |
| 36:1:2225:U:H2'    | 36:1:2226:U:C6     | 2.47                     | 0.50              |
| 36:1:2310:U:OP1    | 86:1:4142:OHX:N1   | 2.45                     | 0.50              |
| 36:1:2505:U:H2'    | 36:1:2506:U:C6     | 2.46                     | 0.50              |
| 86:1:4071:OHX:N1   | 86:1:4118:OHX:N2   | 2.59                     | 0.50              |
| 38:4:14:C:H5'      | 53:M7:121:GLN:O    | 2.12                     | 0.50              |
| 40:L3:350:ALA:O    | 40:L3:351:LEU:HB2  | 2.11                     | 0.50              |
| 41:L4:269:SER:C    | 41:L4:271:LYS:H    | 2.16                     | 0.50              |
| 45:L8:54:GLU:O     | 45:L8:58:VAL:HG23  | 2.12                     | 0.50              |
| 45:L8:130:TYR:CD1  | 45:L8:202:GLU:HB3  | 2.46                     | 0.50              |
| 46:L9:90:MET:HG2   | 46:L9:181:VAL:HG22 | 1.94                     | 0.50              |
| 50:M4:38:ILE:HD11  | 56:N0:150:PHE:CE2  | 2.47                     | 0.50              |
| 1:6:197:A:H61      | 10:s8:138:ASN:HD22 | 1.60                     | 0.50              |
| 1:6:1258:U:H5      | 1:6:1259:U:C2      | 2.30                     | 0.50              |
| 2:s0:66:ALA:HB2    | 23:d1:37:ALA:HB2   | 1.94                     | 0.50              |
| 8:s6:2:LYS:HE2     | 8:s6:17:GLU:OE2    | 2.12                     | 0.50              |
| 8:s6:148:SER:O     | 8:s6:151:ASP:HB2   | 2.11                     | 0.50              |
| 14:c2:45:LEU:H     | 14:c2:120:VAL:HG23 | 1.77                     | 0.50              |
| 25:d3:73:ARG:HE    | 25:d3:84:THR:HG22  | 1.77                     | 0.50              |
| 26:d4:19:ALA:HB1   | 26:d4:81:GLU:OE2   | 2.12                     | 0.50              |
| 28:d6:12:LYS:HE2   | 28:d6:16:GLY:H     | 1.77                     | 0.50              |
| 29:d7:37:CYS:HA    | 29:d7:77:THR:HG22  | 1.92                     | 0.50              |
| 34:sR:25:THR:HA    | 34:sR:73:LEU:HD12  | 1.94                     | 0.50              |
| 34:sR:115:ILE:HG13 | 34:sR:121:MET:O    | 2.12                     | 0.50              |
| 36:5:273:A:N7      | 86:5:4065:OHX:N3   | 2.60                     | 0.50              |
| 36:5:3243:A:OP1    | 52:m6:159:LYS:NZ   | 2.45                     | 0.50              |
| 41:l4:226:GLU:CD   | 41:l4:246:ARG:HH22 | 2.20                     | 0.50              |
| 43:l6:58:LEU:HD12  | 43:l6:78:ARG:HD3   | 1.94                     | 0.50              |
| 45:l8:136:LEU:HD13 | 51:m5:3:ALA:CB     | 2.42                     | 0.50              |
| 62:n6:56:VAL:HG11  | 62:n6:104:LEU:HD13 | 1.93                     | 0.50              |
| 66:o0:99:ASP:O     | 66:o0:101:LEU:N    | 2.44                     | 0.50              |
| 1:2:968:U:H2'      | 1:2:969:C:O4'      | 2.12                     | 0.50              |
| 1:2:1041:G:OP1     | 86:2:2150:OHX:N5   | 2.45                     | 0.50              |
| 2:S0:82:GLY:O      | 2:S0:86:VAL:HG22   | 2.11                     | 0.50              |
| 24:D2:11:LEU:HD12  | 24:D2:74:VAL:HB    | 1.93                     | 0.50              |
| 24:D2:73:GLY:HA3   | 24:D2:128:PHE:CZ   | 2.47                     | 0.50              |
| 36:1:239:G:O2'     | 36:1:240:U:OP1     | 2.26                     | 0.50              |
| 36:1:861:C:H2'     | 36:1:862:U:C6      | 2.47                     | 0.50              |
| 36:1:1492:G:N7     | 75:O9:2:ALA:HB1    | 2.26                     | 0.50              |
| 59:N3:81:GLN:O     | 59:N3:98:ASN:ND2   | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:O0:100:ILE:HD12 | 66:O0:101:LEU:HD23 | 1.93                     | 0.50              |
| 73:O7:21:ARG:HD2   | 73:O7:37:CYS:SG    | 2.52                     | 0.50              |
| 1:6:1796:C:OP2     | 28:d6:92:ARG:HD2   | 2.11                     | 0.50              |
| 2:s0:64:ILE:HG23   | 2:s0:73:VAL:HG11   | 1.93                     | 0.50              |
| 3:s1:173:THR:O     | 3:s1:177:GLN:HB2   | 2.11                     | 0.50              |
| 8:s6:67:VAL:CG2    | 8:s6:99:GLY:HA2    | 2.42                     | 0.50              |
| 17:c5:22:LEU:HA    | 17:c5:25:LEU:HB2   | 1.92                     | 0.50              |
| 19:c7:24:LEU:HD13  | 19:c7:58:MET:HE3   | 1.92                     | 0.50              |
| 25:d3:23:ARG:HH11  | 25:d3:23:ARG:CG    | 2.18                     | 0.50              |
| 26:d4:20:ARG:HH11  | 26:d4:22:GLN:NE2   | 2.10                     | 0.50              |
| 36:5:1221:A:H3'    | 36:5:1222:G:H5'    | 1.94                     | 0.50              |
| 36:5:1919:G:N7     | 86:5:4072:OHX:N4   | 2.59                     | 0.50              |
| 36:5:2592:G:H4'    | 36:5:2594:C:C2     | 2.47                     | 0.50              |
| 48:m1:28:ASP:OD2   | 48:m1:32:ARG:NH2   | 2.44                     | 0.50              |
| 2:S0:189:VAL:HG13  | 2:S0:190:ASP:N     | 2.26                     | 0.50              |
| 4:S2:111:VAL:O     | 4:S2:136:VAL:HA    | 2.12                     | 0.50              |
| 9:S7:41:LEU:HD13   | 9:S7:70:PHE:CD1    | 2.47                     | 0.50              |
| 36:1:3348:G:H1     | 36:1:3357:U:H3     | 1.58                     | 0.50              |
| 86:1:3964:OHX:N1   | 86:1:4143:OHX:N4   | 2.60                     | 0.50              |
| 86:1:4023:OHX:N6   | 86:1:4061:OHX:N2   | 2.60                     | 0.50              |
| 40:L3:138:ALA:O    | 40:L3:140:ASP:N    | 2.44                     | 0.50              |
| 42:L5:155:THR:HA   | 42:L5:179:ARG:HA   | 1.93                     | 0.50              |
| 49:M3:2:ALA:HB2    | 64:N8:31:GLY:O     | 2.12                     | 0.50              |
| 49:M3:47:ALA:HB1   | 49:M3:48:PRO:HD2   | 1.93                     | 0.50              |
| 52:M6:193:GLN:O    | 52:M6:196:ALA:HB3  | 2.11                     | 0.50              |
| 53:M7:48:LEU:HB3   | 53:M7:88:VAL:HG13  | 1.93                     | 0.50              |
| 76:Q0:77:ILE:HG22  | 76:Q0:78:ILE:N     | 2.26                     | 0.50              |
| 1:6:540:G:O2'      | 1:6:542:A:H5'      | 2.11                     | 0.50              |
| 1:6:587:C:H2'      | 1:6:588:U:O4'      | 2.12                     | 0.50              |
| 1:6:765:G:C5       | 11:s9:149:ARG:CZ   | 2.94                     | 0.50              |
| 1:6:1389:C:O2'     | 19:c7:52:GLY:HA3   | 2.12                     | 0.50              |
| 18:c6:82:ARG:NH1   | 18:c6:114:ARG:O    | 2.45                     | 0.50              |
| 36:5:23:A:OP1      | 86:5:3906:OHX:N4   | 2.45                     | 0.50              |
| 36:5:256:G:H2'     | 36:5:257:U:C6      | 2.47                     | 0.50              |
| 36:5:576:C:OP1     | 44:l7:241:LYS:NZ   | 2.44                     | 0.50              |
| 36:5:1554:U:H4'    | 36:5:1555:U:OP1    | 2.10                     | 0.50              |
| 36:5:1556:C:H2'    | 36:5:2169:G:N1     | 2.26                     | 0.50              |
| 36:5:2968:G:N7     | 39:l2:215:ASN:HB2  | 2.27                     | 0.50              |
| 86:5:4000:OHX:N4   | 86:5:4190:OHX:N3   | 2.60                     | 0.50              |
| 37:7:119:U:OP1     | 42:l5:256:THR:HG23 | 2.11                     | 0.50              |
| 43:l6:176:PHE:C    | 50:m4:114:ASP:H    | 2.20                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:m4:50:LYS:HD2   | 50:m4:91:CYS:SG   | 2.52                     | 0.50              |
| 1:2:256:A:H2'      | 1:2:257:A:O4'     | 2.12                     | 0.50              |
| 1:2:872:G:O6       | 86:2:2127:OHX:N3  | 2.45                     | 0.50              |
| 1:2:1553:G:O2'     | 31:D9:14:TYR:OH   | 2.30                     | 0.50              |
| 3:S1:133:TYR:CE1   | 3:S1:220:GLN:HB3  | 2.47                     | 0.50              |
| 3:S1:175:GLU:O     | 3:S1:187:LYS:NZ   | 2.44                     | 0.50              |
| 10:S8:37:LYS:H     | 10:S8:59:ARG:H    | 1.60                     | 0.50              |
| 14:C2:139:HIS:ND1  | 14:C2:139:HIS:O   | 2.45                     | 0.50              |
| 36:1:307:A:O2'     | 36:1:2223:A:N3    | 2.39                     | 0.50              |
| 36:1:956:U:OP1     | 86:1:4128:OHX:N1  | 2.45                     | 0.50              |
| 36:1:1240:A:H3'    | 36:1:1241:U:C5'   | 2.42                     | 0.50              |
| 36:1:1564:U:H2'    | 36:1:1565:G:H8    | 1.76                     | 0.50              |
| 36:1:2339:C:P      | 59:N3:48:ARG:HG2  | 2.52                     | 0.50              |
| 59:N3:86:ARG:HG3   | 59:N3:92:PHE:CE2  | 2.47                     | 0.50              |
| 63:N7:78:ASN:OD1   | 66:O0:35:ARG:NH2  | 2.39                     | 0.50              |
| 66:O0:13:LYS:O     | 66:O0:17:VAL:HG23 | 2.12                     | 0.50              |
| 69:O3:30:ILE:HB    | 69:O3:81:VAL:HG12 | 1.93                     | 0.50              |
| 70:O4:58:ARG:HH11  | 70:O4:58:ARG:CG   | 2.24                     | 0.50              |
| 71:O5:101:THR:HG23 | 71:O5:103:LYS:H   | 1.77                     | 0.50              |
| 1:6:934:C:H6       | 28:d6:11:ASN:HB3  | 1.75                     | 0.50              |
| 1:6:1429:G:H2'     | 1:6:1430:U:C6     | 2.46                     | 0.50              |
| 1:6:1434:U:H4'     | 31:d9:24:CYS:HB2  | 1.94                     | 0.50              |
| 1:6:1487:A:OP1     | 31:d9:34:TYR:OH   | 2.22                     | 0.50              |
| 1:6:1727:G:H2'     | 1:6:1728:A:C8     | 2.47                     | 0.50              |
| 3:s1:135:LEU:HD21  | 3:s1:217:LEU:HD12 | 1.94                     | 0.50              |
| 6:s4:98:ASN:ND2    | 6:s4:116:ASP:OD1  | 2.45                     | 0.50              |
| 7:s5:159:ALA:HB3   | 7:s5:225:ARG:HB3  | 1.94                     | 0.50              |
| 11:s9:109:LEU:HB2  | 11:s9:146:PHE:CB  | 2.41                     | 0.50              |
| 11:s9:120:LYS:O    | 11:s9:120:LYS:HD3 | 2.12                     | 0.50              |
| 21:c9:112:GLY:O    | 21:c9:127:ASN:HB3 | 2.12                     | 0.50              |
| 36:5:1688:U:H2'    | 36:5:1689:U:C5    | 2.46                     | 0.50              |
| 36:5:1758:G:H5'    | 58:n2:104:ARG:NH2 | 2.27                     | 0.50              |
| 86:5:4055:OHX:N1   | 86:5:4197:OHX:N4  | 2.60                     | 0.50              |
| 39:l2:214:GLY:O    | 39:l2:215:ASN:HB2 | 2.11                     | 0.50              |
| 40:l3:332:ARG:O    | 40:l3:333:LYS:HB2 | 2.12                     | 0.50              |
| 41:l4:60:THR:HG21  | 41:l4:77:VAL:HG22 | 1.94                     | 0.50              |
| 41:l4:319:LYS:O    | 41:l4:320:ASN:HB3 | 2.12                     | 0.50              |
| 46:l9:75:VAL:HA    | 46:l9:78:MET:HE3  | 1.93                     | 0.50              |
| 63:n7:124:ALA:O    | 63:n7:126:LYS:N   | 2.45                     | 0.50              |
| 65:n9:20:GLY:O     | 65:n9:21:ILE:HB   | 2.10                     | 0.50              |
| 1:2:197:A:H2'      | 1:2:198:A:C8      | 2.46                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:495:C:H3'     | 1:2:496:G:O4'      | 2.11                     | 0.49              |
| 1:2:569:C:H41     | 25:D3:69:ARG:NH1   | 2.10                     | 0.49              |
| 1:2:856:A:N7      | 9:S7:97:ARG:HB2    | 2.28                     | 0.49              |
| 1:2:1535:U:O2'    | 1:2:1536:G:H5''    | 2.12                     | 0.49              |
| 3:S1:56:SER:OG    | 3:S1:59:ASP:OD1    | 2.30                     | 0.49              |
| 11:S9:38:ASN:HB2  | 11:S9:41:GLU:HG3   | 1.93                     | 0.49              |
| 15:C3:11:ILE:O    | 15:C3:11:ILE:HG12  | 2.12                     | 0.49              |
| 24:D2:111:MET:HE3 | 24:D2:116:ALA:HA   | 1.93                     | 0.49              |
| 30:D8:9:LEU:HD13  | 30:D8:53:ILE:HG21  | 1.94                     | 0.49              |
| 34:SR:161:LYS:HD3 | 34:SR:164:ASP:HB3  | 1.93                     | 0.49              |
| 36:1:269:G:O6     | 86:1:4083:OHX:N3   | 2.45                     | 0.49              |
| 36:1:1581:C:H2'   | 36:1:1582:C:C5'    | 2.42                     | 0.49              |
| 47:M0:174:THR:CG2 | 47:M0:176:LEU:H    | 2.11                     | 0.49              |
| 52:M6:61:ALA:HA   | 52:M6:70:PRO:HD2   | 1.94                     | 0.49              |
| 59:N3:80:ARG:NH1  | 59:N3:116:GLY:HA3  | 2.27                     | 0.49              |
| 66:O0:46:ALA:HB2  | 66:O0:72:GLY:H     | 1.76                     | 0.49              |
| 1:6:190:C:O2'     | 1:6:191:C:O5'      | 2.30                     | 0.49              |
| 1:6:747:C:O2'     | 24:d2:124:LYS:HE2  | 2.11                     | 0.49              |
| 1:6:1600:A:H4'    | 1:6:1601:G:OP1     | 2.11                     | 0.49              |
| 11:s9:27:GLU:OE1  | 11:s9:39:LYS:NZ    | 2.40                     | 0.49              |
| 36:5:913:A:H2     | 36:5:2134:G:N3     | 2.10                     | 0.49              |
| 36:5:992:A:O2'    | 36:5:993:G:H5'     | 2.12                     | 0.49              |
| 38:8:83:C:H4'     | 38:8:85:G:C2       | 2.47                     | 0.49              |
| 40:l3:169:THR:CG2 | 40:l3:171:LEU:H    | 2.25                     | 0.49              |
| 47:m0:142:ASP:CG  | 47:m0:178:ARG:HH22 | 2.20                     | 0.49              |
| 47:m0:208:ASN:HA  | 47:m0:211:ARG:HD2  | 1.94                     | 0.49              |
| 59:n3:66:LYS:O    | 59:n3:70:ARG:HG3   | 2.12                     | 0.49              |
| 60:n4:120:LYS:O   | 60:n4:123:ARG:HB2  | 2.12                     | 0.49              |
| 74:o8:16:ARG:O    | 74:o8:18:ALA:N     | 2.44                     | 0.49              |
| 1:2:56:U:H4'      | 1:2:57:G:H5'       | 1.94                     | 0.49              |
| 1:2:856:A:H1'     | 9:S7:64:VAL:HG11   | 1.94                     | 0.49              |
| 1:2:1171:A:H2'    | 1:2:1172:G:C8      | 2.46                     | 0.49              |
| 1:2:1351:G:C2     | 1:2:1375:A:C2      | 3.00                     | 0.49              |
| 1:2:1794:A:H1'    | 28:D6:79:ILE:HD13  | 1.93                     | 0.49              |
| 11:S9:34:PHE:HD1  | 11:S9:111:THR:HG21 | 1.77                     | 0.49              |
| 11:S9:126:ARG:O   | 11:S9:130:THR:HG22 | 2.12                     | 0.49              |
| 12:C0:49:LEU:O    | 12:C0:54:TYR:HB2   | 2.12                     | 0.49              |
| 27:D5:60:VAL:HG22 | 27:D5:101:TYR:HB2  | 1.93                     | 0.49              |
| 29:D7:54:VAL:O    | 29:D7:63:LEU:HB2   | 2.12                     | 0.49              |
| 34:SR:267:PRO:HG2 | 34:SR:269:TYR:CE1  | 2.47                     | 0.49              |
| 36:1:1480:G:H4'   | 36:1:1481:A:OP1    | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1722:U:OP1    | 55:M9:100:ARG:HD3  | 2.12                     | 0.49              |
| 36:1:2655:U:OP2    | 78:Q2:2:VAL:HA     | 2.12                     | 0.49              |
| 86:1:4059:OHX:N6   | 86:1:4166:OHX:N3   | 2.60                     | 0.49              |
| 39:L2:130:SER:HA   | 39:L2:169:ILE:HG22 | 1.93                     | 0.49              |
| 40:L3:347:SER:O    | 40:L3:348:ARG:HB3  | 2.12                     | 0.49              |
| 50:M4:89:ALA:HB1   | 50:M4:92:GLU:CD    | 2.37                     | 0.49              |
| 67:O1:13:THR:HG22  | 67:O1:72:ARG:HH11  | 1.77                     | 0.49              |
| 74:O8:32:ASN:O     | 74:O8:34:ALA:N     | 2.45                     | 0.49              |
| 1:6:219:A:N6       | 1:6:843:U:C2       | 2.79                     | 0.49              |
| 1:6:484:C:H42      | 1:6:503:G:N2       | 2.10                     | 0.49              |
| 1:6:1255:G:O2'     | 1:6:1256:A:O5'     | 2.29                     | 0.49              |
| 3:s1:125:VAL:HG11  | 3:s1:173:THR:HG22  | 1.93                     | 0.49              |
| 5:s3:64:ARG:O      | 5:s3:66:ILE:N      | 2.41                     | 0.49              |
| 5:s3:115:ILE:HD12  | 5:s3:116:ARG:H     | 1.77                     | 0.49              |
| 17:c5:126:VAL:HG22 | 17:c5:127:ARG:H    | 1.77                     | 0.49              |
| 21:c9:131:ASP:OD2  | 21:c9:134:ARG:NH1  | 2.45                     | 0.49              |
| 34:sR:38:ARG:HG2   | 34:sR:67:ILE:CG2   | 2.41                     | 0.49              |
| 36:5:1409:G:N7     | 86:5:4160:OHX:N6   | 2.60                     | 0.49              |
| 36:5:1764:U:H3'    | 36:5:1765:U:C5'    | 2.43                     | 0.49              |
| 36:5:2822:U:OP2    | 86:5:3953:OHX:N1   | 2.45                     | 0.49              |
| 36:5:2943:G:H2'    | 36:5:2944:U:O4'    | 2.11                     | 0.49              |
| 86:5:3973:OHX:N1   | 86:5:4241:OHX:N2   | 2.60                     | 0.49              |
| 39:l2:24:GLN:OE1   | 39:l2:60:LYS:NZ    | 2.44                     | 0.49              |
| 40:l3:265:ALA:C    | 40:l3:266:ARG:HG2  | 2.37                     | 0.49              |
| 47:m0:36:LEU:HD22  | 47:m0:73:ASN:ND2   | 2.27                     | 0.49              |
| 52:m6:56:ASP:O     | 52:m6:59:ARG:HG2   | 2.12                     | 0.49              |
| 57:n1:68:THR:HG22  | 57:n1:71:SER:O     | 2.12                     | 0.49              |
| 62:n6:102:SER:OG   | 62:n6:103:LYS:HE2  | 2.12                     | 0.49              |
| 1:2:583:C:OP1      | 86:2:2027:OHX:N3   | 2.45                     | 0.49              |
| 1:2:1553:G:O6      | 17:C5:43:ARG:HD3   | 2.12                     | 0.49              |
| 9:S7:67:LEU:HD13   | 9:S7:71:HIS:CE1    | 2.47                     | 0.49              |
| 10:S8:197:THR:C    | 10:S8:199:LYS:H    | 2.20                     | 0.49              |
| 15:C3:115:LEU:HD22 | 15:C3:119:GLU:HG3  | 1.94                     | 0.49              |
| 36:1:801:A:O2'     | 86:1:3985:OHX:N2   | 2.45                     | 0.49              |
| 36:1:1192:C:O2     | 86:1:4054:OHX:N3   | 2.44                     | 0.49              |
| 36:1:1230:G:H2'    | 36:1:1231:A:H8     | 1.77                     | 0.49              |
| 36:1:1629:U:P      | 63:N7:112:LYS:HE2  | 2.52                     | 0.49              |
| 36:1:1752:A:OP2    | 86:1:4051:OHX:N5   | 2.45                     | 0.49              |
| 36:1:2366:C:H5'    | 40:L3:259:HIS:HE2  | 1.77                     | 0.49              |
| 36:1:2631:U:OP1    | 36:1:2757:U:O2'    | 2.30                     | 0.49              |
| 36:1:2943:G:C8     | 40:L3:2:SER:N      | 2.80                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:1:3096:C:H2'   | 36:1:3097:C:C6    | 2.47                     | 0.49              |
| 51:M5:183:THR:O   | 51:M5:184:LYS:HB2 | 2.12                     | 0.49              |
| 1:6:448:C:OP1     | 6:s4:29:PRO:HD3   | 2.12                     | 0.49              |
| 1:6:629:U:OP1     | 15:c3:127:ARG:NH2 | 2.45                     | 0.49              |
| 7:s5:63:GLN:HB3   | 7:s5:88:PRO:HA    | 1.93                     | 0.49              |
| 36:5:420:G:OP2    | 36:5:420:G:OP1    | 2.30                     | 0.49              |
| 36:5:911:C:N4     | 39:l2:3:ARG:HD3   | 2.25                     | 0.49              |
| 36:5:1222:G:O6    | 86:5:4128:OHX:N1  | 2.46                     | 0.49              |
| 36:5:1734:G:O6    | 86:5:3969:OHX:N5  | 2.46                     | 0.49              |
| 36:5:1769:G:C2    | 36:5:1770:G:C8    | 3.00                     | 0.49              |
| 36:5:2157:G:O3'   | 39:l2:156:LYS:NZ  | 2.45                     | 0.49              |
| 36:5:3228:C:H4'   | 36:5:3229:G:O5'   | 2.11                     | 0.49              |
| 52:m6:110:PRO:C   | 52:m6:112:TYR:N   | 2.71                     | 0.49              |
| 67:o1:83:GLU:O    | 67:o1:85:ALA:N    | 2.45                     | 0.49              |
| 68:o2:41:VAL:HG12 | 68:o2:46:PHE:CD2  | 2.47                     | 0.49              |
| 9:S7:23:ALA:O     | 9:S7:27:LEU:HG    | 2.12                     | 0.49              |
| 10:S8:8:ARG:HG3   | 10:S8:8:ARG:O     | 2.12                     | 0.49              |
| 18:C6:41:PRO:O    | 18:C6:43:ILE:N    | 2.41                     | 0.49              |
| 20:C8:30:TYR:O    | 20:C8:33:THR:OG1  | 2.28                     | 0.49              |
| 23:D1:38:LYS:HD3  | 23:D1:51:VAL:HG23 | 1.94                     | 0.49              |
| 29:D7:47:PHE:CE1  | 29:D7:49:HIS:HB2  | 2.47                     | 0.49              |
| 31:D9:5:ASN:C     | 31:D9:7:TRP:H     | 2.21                     | 0.49              |
| 36:1:784:A:C6     | 54:M8:93:ILE:HG22 | 2.48                     | 0.49              |
| 36:1:1014:U:C2'   | 36:1:1015:U:H5''  | 2.42                     | 0.49              |
| 36:1:1104:G:H8    | 36:1:1104:G:O5'   | 1.95                     | 0.49              |
| 86:1:3980:OHX:N5  | 86:1:4158:OHX:N2  | 2.60                     | 0.49              |
| 38:4:10:A:H2'     | 38:4:11:C:C6      | 2.47                     | 0.49              |
| 40:L3:35:ASP:OD1  | 40:L3:184:ASN:O   | 2.31                     | 0.49              |
| 47:M0:31:ILE:HG13 | 47:M0:32:ARG:N    | 2.27                     | 0.49              |
| 49:M3:80:VAL:HG12 | 49:M3:85:LEU:O    | 2.12                     | 0.49              |
| 56:N0:46:GLN:HG2  | 56:N0:51:VAL:O    | 2.11                     | 0.49              |
| 63:N7:135:ARG:HG2 | 63:N7:135:ARG:NH2 | 2.22                     | 0.49              |
| 67:O1:13:THR:CG2  | 67:O1:72:ARG:HH11 | 2.25                     | 0.49              |
| 72:O6:93:ILE:O    | 72:O6:97:SER:HB3  | 2.12                     | 0.49              |
| 1:6:1401:A:OP1    | 19:c7:60:ARG:NH1  | 2.46                     | 0.49              |
| 86:6:2060:OHX:N5  | 86:6:2147:OHX:N3  | 2.60                     | 0.49              |
| 86:6:2118:OHX:N3  | 59:n3:133:SER:O   | 2.45                     | 0.49              |
| 3:s1:103:MET:HB3  | 3:s1:215:VAL:CG1  | 2.42                     | 0.49              |
| 18:c6:82:ARG:HH12 | 18:c6:114:ARG:HB2 | 1.77                     | 0.49              |
| 20:c8:56:LYS:HD2  | 20:c8:61:LEU:HD23 | 1.94                     | 0.49              |
| 36:5:8:C:H2'      | 36:5:9:U:O4'      | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:5:1595:U:C2    | 36:5:1596:C:C5     | 3.00                     | 0.49              |
| 36:5:2722:U:OP1   | 65:n9:33:LYS:NZ    | 2.45                     | 0.49              |
| 36:5:3047:U:O2'   | 40:l3:53:MET:HE1   | 2.12                     | 0.49              |
| 36:5:3121:U:H1'   | 36:5:3122:A:H5''   | 1.94                     | 0.49              |
| 38:8:62:C:O2      | 86:8:219:OHX:N1    | 2.45                     | 0.49              |
| 41:l4:255:PHE:O   | 41:l4:258:LEU:HB2  | 2.12                     | 0.49              |
| 1:2:2:A:C2        | 4:S2:170:ILE:HD12  | 2.47                     | 0.49              |
| 1:2:990:C:H2'     | 1:2:991:G:O4'      | 2.12                     | 0.49              |
| 2:S0:9:LEU:HD23   | 2:S0:54:TRP:CG     | 2.48                     | 0.49              |
| 3:S1:171:ILE:HD13 | 3:S1:196:GLU:HG2   | 1.95                     | 0.49              |
| 4:S2:53:ILE:HD11  | 4:S2:73:LEU:HD22   | 1.94                     | 0.49              |
| 7:S5:41:LYS:O     | 7:S5:67:PRO:HB2    | 2.12                     | 0.49              |
| 8:S6:67:VAL:O     | 8:S6:68:LEU:HB2    | 2.13                     | 0.49              |
| 11:S9:117:GLY:C   | 11:S9:119:ALA:H    | 2.21                     | 0.49              |
| 12:C0:32:HIS:CD2  | 12:C0:35:ILE:HB    | 2.47                     | 0.49              |
| 15:C3:89:TYR:CE2  | 15:C3:150:VAL:HG22 | 2.47                     | 0.49              |
| 28:D6:44:ILE:HD12 | 28:D6:45:VAL:N     | 2.27                     | 0.49              |
| 35:SM:70:ASN:O    | 35:SM:74:LYS:HD3   | 2.12                     | 0.49              |
| 36:1:174:C:H2'    | 36:1:175:C:C6      | 2.47                     | 0.49              |
| 36:1:190:U:H2'    | 62:N6:60:ARG:NH2   | 2.26                     | 0.49              |
| 36:1:2437:G:N2    | 36:1:2511:A:H1'    | 2.27                     | 0.49              |
| 36:1:2611:U:H2'   | 36:1:2612:U:C6     | 2.47                     | 0.49              |
| 36:1:2790:A:OP2   | 54:M8:181:SER:HB3  | 2.12                     | 0.49              |
| 42:L5:50:ARG:NH2  | 42:L5:147:ASP:OD2  | 2.37                     | 0.49              |
| 44:L7:96:PRO:HB2  | 44:L7:99:PRO:HD2   | 1.95                     | 0.49              |
| 47:M0:51:HIS:CD2  | 57:N1:160:ILE:HG23 | 2.46                     | 0.49              |
| 49:M3:57:VAL:HG12 | 49:M3:58:VAL:H     | 1.78                     | 0.49              |
| 1:6:1250:U:O2'    | 33:e1:135:HIS:HB3  | 2.12                     | 0.49              |
| 1:6:1341:A:O2'    | 34:sR:102:ARG:NH2  | 2.45                     | 0.49              |
| 1:6:1491:U:H5'    | 1:6:1492:A:OP1     | 2.11                     | 0.49              |
| 86:6:2060:OHX:N2  | 86:6:2147:OHX:N6   | 2.60                     | 0.49              |
| 8:s6:31:ARG:HH11  | 8:s6:34:GLN:NE2    | 2.08                     | 0.49              |
| 9:s7:140:VAL:HG22 | 9:s7:150:GLN:HG2   | 1.94                     | 0.49              |
| 18:c6:12:LYS:HE2  | 18:c6:17:THR:HB    | 1.94                     | 0.49              |
| 36:5:211:A:OP1    | 41:l4:220:ARG:NH1  | 2.41                     | 0.49              |
| 36:5:419:G:N7     | 86:8:214:OHX:N3    | 2.61                     | 0.49              |
| 36:5:595:G:N1     | 36:5:609:G:H5''    | 2.28                     | 0.49              |
| 36:5:1072:G:H2'   | 36:5:1073:U:H6     | 1.77                     | 0.49              |
| 36:5:1505:C:OP1   | 53:m7:127:ARG:HD2  | 2.13                     | 0.49              |
| 36:5:2635:A:H4'   | 36:5:2636:A:O5'    | 2.12                     | 0.49              |
| 39:l2:225:ILE:O   | 39:l2:238:ILE:O    | 2.30                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:m6:8:VAL:HG13   | 52:m6:34:VAL:HG22  | 1.94                     | 0.49              |
| 70:o4:16:ARG:HH11  | 70:o4:16:ARG:CG    | 2.24                     | 0.49              |
| 73:o7:16:HIS:HA    | 73:o7:27:PHE:O     | 2.12                     | 0.49              |
| 1:2:1055:U:O4      | 86:2:2166:OHX:N3   | 2.46                     | 0.49              |
| 1:2:1102:G:P       | 24:D2:76:SER:HB2   | 2.53                     | 0.49              |
| 1:2:1173:C:OP1     | 20:C8:132:ARG:NH1  | 2.46                     | 0.49              |
| 1:2:1291:G:O5'     | 1:2:1291:G:H8      | 1.96                     | 0.49              |
| 1:2:1786:G:P       | 16:C4:136:ARG:HH22 | 2.35                     | 0.49              |
| 9:S7:41:LEU:HB3    | 9:S7:70:PHE:CE1    | 2.47                     | 0.49              |
| 15:C3:15:ALA:HB2   | 29:D7:20:LYS:HG3   | 1.93                     | 0.49              |
| 21:C9:45:MET:HE3   | 21:C9:46:PRO:HD2   | 1.94                     | 0.49              |
| 36:1:92:G:OP2      | 36:1:93:C:H5''     | 2.12                     | 0.49              |
| 36:1:156:G:OP2     | 72:O6:25:LYS:HB3   | 2.12                     | 0.49              |
| 36:1:709:A:P       | 54:M8:179:ARG:HH22 | 2.32                     | 0.49              |
| 36:1:898:U:H2'     | 36:1:899:U:O4'     | 2.13                     | 0.49              |
| 36:1:1352:A:H1'    | 36:1:1353:U:O5'    | 2.13                     | 0.49              |
| 36:1:1460:A:H2'    | 36:1:1461:A:H8     | 1.77                     | 0.49              |
| 36:1:1615:C:H2'    | 36:1:1616:U:C6     | 2.48                     | 0.49              |
| 36:1:1658:G:H2'    | 36:1:1659:U:C6     | 2.48                     | 0.49              |
| 36:1:2880:U:H1'    | 40:L3:250:ALA:HB3  | 1.93                     | 0.49              |
| 45:L8:203:VAL:HG13 | 45:L8:204:ARG:O    | 2.12                     | 0.49              |
| 54:M8:24:VAL:HG23  | 54:M8:25:TYR:CD2   | 2.47                     | 0.49              |
| 55:M9:115:ILE:HG12 | 55:M9:119:LEU:HD23 | 1.95                     | 0.49              |
| 57:N1:56:PHE:CE1   | 57:N1:78:LYS:HD3   | 2.47                     | 0.49              |
| 57:N1:105:PHE:O    | 57:N1:108:ARG:N    | 2.45                     | 0.49              |
| 66:O0:45:ALA:HB3   | 66:O0:48:THR:HG22  | 1.94                     | 0.49              |
| 73:O7:48:ASN:OD1   | 73:O7:54:LYS:NZ    | 2.45                     | 0.49              |
| 74:O8:62:ALA:O     | 74:O8:66:ILE:HG13  | 2.13                     | 0.49              |
| 1:6:496:G:O6       | 1:6:497:G:N2       | 2.42                     | 0.49              |
| 1:6:825:U:O2'      | 1:6:826:U:OP2      | 2.24                     | 0.49              |
| 11:s9:118:LEU:HD23 | 11:s9:158:PHE:CZ   | 2.47                     | 0.49              |
| 11:s9:129:ILE:HA   | 11:s9:134:ILE:CG1  | 2.43                     | 0.49              |
| 30:d8:60:GLU:O     | 30:d8:62:GLU:N     | 2.45                     | 0.49              |
| 36:5:731:U:H2'     | 36:5:732:C:H6      | 1.77                     | 0.49              |
| 36:5:789:A:H2'     | 36:5:790:U:C6      | 2.47                     | 0.49              |
| 36:5:926:A:H2'     | 36:5:927:C:C6      | 2.47                     | 0.49              |
| 36:5:2726:C:O2'    | 36:5:2727:A:H2'    | 2.13                     | 0.49              |
| 43:l6:98:VAL:HA    | 43:l6:101:PHE:CD2  | 2.48                     | 0.49              |
| 73:o7:48:ASN:HA    | 73:o7:54:LYS:HZ2   | 1.77                     | 0.49              |
| 1:2:217:A:OP1      | 1:2:217:A:H2'      | 2.13                     | 0.49              |
| 1:2:1022:C:H4'     | 1:2:1125:A:H61     | 1.76                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1282:U:OP1     | 86:2:2115:OHX:N5   | 2.46                     | 0.49              |
| 4:S2:38:VAL:O      | 4:S2:39:THR:OG1    | 2.30                     | 0.49              |
| 9:S7:174:ASN:O     | 9:S7:178:GLY:N     | 2.45                     | 0.49              |
| 11:S9:65:LYS:HA    | 11:S9:70:LEU:HG    | 1.93                     | 0.49              |
| 15:C3:151:ASN:O    | 86:C3:202:OHX:N6   | 2.46                     | 0.49              |
| 34:SR:90:ARG:NH1   | 34:SR:99:THR:OG1   | 2.45                     | 0.49              |
| 36:1:1580:A:H5'    | 36:1:2522:G:N7     | 2.27                     | 0.49              |
| 36:1:2405:C:O2     | 36:1:2819:A:N1     | 2.46                     | 0.49              |
| 36:1:2513:U:H2'    | 36:1:2592:G:N1     | 2.25                     | 0.49              |
| 36:1:2539:C:H5'    | 36:1:2541:U:O4     | 2.13                     | 0.49              |
| 86:1:3955:OHX:N2   | 86:1:4041:OHX:N6   | 2.61                     | 0.49              |
| 38:4:68:G:OP2      | 86:O7:103:OHX:N6   | 2.45                     | 0.49              |
| 39:L2:209:HIS:HD2  | 39:L2:211:HIS:N    | 2.01                     | 0.49              |
| 41:L4:292:SER:OG   | 41:L4:293:SER:N    | 2.45                     | 0.49              |
| 42:L5:131:LEU:HD22 | 42:L5:131:LEU:H    | 1.77                     | 0.49              |
| 43:L6:18:LEU:N     | 43:L6:18:LEU:HD22  | 2.28                     | 0.49              |
| 45:L8:162:LEU:HA   | 51:M5:7:LEU:HD11   | 1.94                     | 0.49              |
| 69:O3:15:SER:OG    | 69:O3:16:TYR:O     | 2.29                     | 0.49              |
| 1:6:151:G:N2       | 8:s6:13:GLN:OE1    | 2.35                     | 0.49              |
| 1:6:327:U:H1'      | 13:c1:10:GLU:HG2   | 1.94                     | 0.49              |
| 1:6:453:U:H3'      | 1:6:453:U:O2       | 2.12                     | 0.49              |
| 1:6:542:A:H1'      | 1:6:543:C:OP1      | 2.13                     | 0.49              |
| 1:6:647:G:H22      | 1:6:687:G:H1       | 1.61                     | 0.49              |
| 1:6:918:U:H2'      | 1:6:919:A:C8       | 2.46                     | 0.49              |
| 1:6:1333:C:H4'     | 5:s3:162:GLN:HG3   | 1.95                     | 0.49              |
| 4:s2:67:GLN:O      | 4:s2:71:THR:HG23   | 2.13                     | 0.49              |
| 6:s4:195:ILE:O     | 6:s4:209:HIS:O     | 2.30                     | 0.49              |
| 34:sR:22:SER:OG    | 34:sR:69:GLN:O     | 2.31                     | 0.49              |
| 36:5:215:G:OP1     | 62:n6:12:ARG:HG2   | 2.12                     | 0.49              |
| 41:l4:35:VAL:HG13  | 41:l4:235:LEU:HD11 | 1.93                     | 0.49              |
| 42:l5:155:THR:HG22 | 42:l5:179:ARG:NH1  | 2.27                     | 0.49              |
| 81:m2:152:UNK:O    | 81:m2:155:UNK:N    | 2.45                     | 0.49              |
| 50:m4:40:ASP:HA    | 56:n0:143:PHE:CE1  | 2.47                     | 0.49              |
| 1:2:79:C:H4'       | 8:S6:173:PRO:O     | 2.12                     | 0.49              |
| 1:2:445:A:H1'      | 1:2:525:A:OP1      | 2.13                     | 0.49              |
| 1:2:699:U:H2'      | 1:2:700:C:C6       | 2.48                     | 0.49              |
| 1:2:886:U:O2'      | 16:C4:121:VAL:O    | 2.29                     | 0.49              |
| 16:C4:122:PRO:C    | 16:C4:124:ASP:N    | 2.70                     | 0.49              |
| 36:1:817:A:H8      | 73:O7:15:SER:HG    | 1.59                     | 0.49              |
| 36:1:1554:U:C2     | 36:1:1555:U:C5     | 3.00                     | 0.49              |
| 86:1:4084:OHX:N4   | 86:1:4153:OHX:N1   | 2.59                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:L3:41:VAL:HA    | 40:L3:185:GLY:CA   | 2.41                     | 0.49              |
| 46:L9:29:GLY:HA3   | 46:L9:82:VAL:HG13  | 1.95                     | 0.49              |
| 47:M0:210:ILE:HG12 | 47:M0:217:PHE:CE2  | 2.48                     | 0.49              |
| 60:N4:34:SER:HA    | 60:N4:37:ALA:HB3   | 1.95                     | 0.49              |
| 62:N6:125:LYS:O    | 62:N6:126:LEU:HG   | 2.12                     | 0.49              |
| 1:6:30:G:H2'       | 1:6:31:C:C6        | 2.46                     | 0.49              |
| 9:s7:73:VAL:O      | 9:s7:75:THR:N      | 2.45                     | 0.49              |
| 9:s7:115:SER:O     | 9:s7:116:ARG:HB2   | 2.11                     | 0.49              |
| 11:s9:92:LYS:HB2   | 11:s9:95:TYR:HD2   | 1.78                     | 0.49              |
| 12:c0:87:VAL:O     | 12:c0:89:ALA:N     | 2.46                     | 0.49              |
| 20:c8:91:ASP:HB3   | 20:c8:95:GLY:H     | 1.78                     | 0.49              |
| 24:d2:23:ARG:HB2   | 29:d7:4:VAL:HG12   | 1.94                     | 0.49              |
| 34:sR:61:PHE:HD1   | 34:sR:92:TRP:CE3   | 2.30                     | 0.49              |
| 36:5:1433:A:P      | 68:o2:19:ARG:HH22  | 2.36                     | 0.49              |
| 36:5:1749:A:H8     | 36:5:1749:A:OP1    | 1.95                     | 0.49              |
| 54:m8:41:ASP:HB2   | 54:m8:42:ALA:H     | 1.44                     | 0.49              |
| 1:2:474:A:O2'      | 11:S9:37:LYS:HE2   | 2.13                     | 0.49              |
| 1:2:1516:A:O2'     | 1:2:1517:U:H5'     | 2.13                     | 0.49              |
| 7:S5:205:SER:C     | 7:S5:207:THR:H     | 2.21                     | 0.49              |
| 9:S7:30:SER:HB3    | 9:S7:34:LEU:HD12   | 1.94                     | 0.49              |
| 11:S9:40:LYS:HA    | 11:S9:43:TYR:HB2   | 1.94                     | 0.49              |
| 20:C8:49:LYS:NZ    | 20:C8:79:TYR:O     | 2.45                     | 0.49              |
| 29:D7:56:CYS:SG    | 29:D7:57:GLU:N     | 2.85                     | 0.49              |
| 36:1:155:G:O2'     | 72:O6:27:SER:HB3   | 2.12                     | 0.49              |
| 36:1:981:U:HO2'    | 36:1:982:C:P       | 2.36                     | 0.49              |
| 36:1:3228:C:H4'    | 36:1:3229:G:O5'    | 2.12                     | 0.49              |
| 36:1:3291:G:O2'    | 36:1:3292:A:H5'    | 2.12                     | 0.49              |
| 46:L9:31:ARG:HH21  | 46:L9:188:THR:HG22 | 1.78                     | 0.49              |
| 49:M3:119:TYR:O    | 49:M3:123:ILE:HG23 | 2.12                     | 0.49              |
| 61:N5:63:ILE:HD13  | 61:N5:63:ILE:O     | 2.13                     | 0.49              |
| 69:O3:23:ASN:OD1   | 69:O3:25:PRO:HD3   | 2.12                     | 0.49              |
| 1:6:162:A:H2'      | 1:6:163:G:C8       | 2.47                     | 0.49              |
| 1:6:230:C:N3       | 1:6:235:G:N2       | 2.50                     | 0.49              |
| 1:6:687:G:H5''     | 24:d2:119:LYS:HG2  | 1.95                     | 0.49              |
| 1:6:846:G:H21      | 13:c1:46:LYS:HE2   | 1.78                     | 0.49              |
| 1:6:894:U:H2'      | 1:6:895:G:C8       | 2.48                     | 0.49              |
| 1:6:1255:G:O2'     | 1:6:1256:A:H8      | 1.96                     | 0.49              |
| 1:6:1563:C:OP1     | 21:c9:84:LYS:HE3   | 2.12                     | 0.49              |
| 3:s1:48:VAL:HG21   | 3:s1:61:LEU:HD13   | 1.95                     | 0.49              |
| 17:c5:37:ALA:O     | 17:c5:42:ARG:NH1   | 2.46                     | 0.49              |
| 34:sR:37:SER:OG    | 34:sR:38:ARG:N     | 2.45                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:5:90:C:C2'     | 36:5:91:G:H5'      | 2.43                     | 0.49              |
| 36:5:96:G:H5''    | 49:m3:15:ARG:CZ    | 2.42                     | 0.49              |
| 36:5:132:C:C2'    | 36:5:133:U:H5''    | 2.42                     | 0.49              |
| 36:5:1062:A:H4'   | 57:n1:105:PHE:CE2  | 2.48                     | 0.49              |
| 36:5:1176:C:H2'   | 36:5:1177:G:N2     | 2.28                     | 0.49              |
| 36:5:1296:C:H5'   | 56:n0:115:ARG:NH1  | 2.28                     | 0.49              |
| 36:5:1555:U:H5'   | 36:5:1556:C:OP2    | 2.13                     | 0.49              |
| 36:5:1588:A:C2    | 75:o9:4:GLN:HG2    | 2.48                     | 0.49              |
| 37:7:2:G:H4'      | 42:l5:270:LYS:HD3  | 1.93                     | 0.49              |
| 49:m3:162:ASN:ND2 | 49:m3:164:GLU:HB2  | 2.27                     | 0.49              |
| 51:m5:47:LYS:HE3  | 51:m5:51:LEU:HD11  | 1.95                     | 0.49              |
| 67:o1:40:ALA:O    | 67:o1:43:HIS:O     | 2.31                     | 0.49              |
| 1:2:138:A:N6      | 1:2:266:A:H61      | 2.11                     | 0.49              |
| 1:2:1316:G:H2'    | 1:2:1317:C:C6      | 2.48                     | 0.49              |
| 2:S0:33:GLN:C     | 2:S0:34:GLU:HG2    | 2.37                     | 0.49              |
| 6:S4:11:ARG:O     | 6:S4:12:LEU:HB2    | 2.12                     | 0.49              |
| 9:S7:161:GLN:O    | 9:S7:165:LYS:HE3   | 2.13                     | 0.49              |
| 14:C2:54:ARG:NH1  | 14:C2:56:GLU:OE2   | 2.44                     | 0.49              |
| 24:D2:23:ARG:NH1  | 24:D2:65:LEU:O     | 2.46                     | 0.49              |
| 36:1:1765:U:H2'   | 36:1:1766:G:H8     | 1.78                     | 0.49              |
| 36:1:2585:G:C6    | 61:N5:24:LEU:HD13  | 2.48                     | 0.49              |
| 36:1:2662:G:H2'   | 36:1:2663:G:C8     | 2.48                     | 0.49              |
| 36:1:2714:G:H4'   | 36:1:2715:A:O5'    | 2.13                     | 0.49              |
| 36:1:3103:A:OP2   | 86:1:4170:OHX:N3   | 2.46                     | 0.49              |
| 86:1:4071:OHX:N5  | 86:1:4118:OHX:N6   | 2.60                     | 0.49              |
| 42:L5:106:ALA:HB2 | 42:L5:166:ALA:HA   | 1.95                     | 0.49              |
| 47:M0:33:ILE:HD11 | 47:M0:36:LEU:HG    | 1.93                     | 0.49              |
| 57:N1:57:TYR:OH   | 57:N1:87:LYS:HD2   | 2.13                     | 0.49              |
| 59:N3:120:LYS:H   | 59:N3:137:VAL:HG23 | 1.78                     | 0.49              |
| 71:O5:6:ALA:O     | 71:O5:9:LEU:N      | 2.46                     | 0.49              |
| 75:O9:9:ILE:HG22  | 75:O9:13:MET:CE    | 2.43                     | 0.49              |
| 1:6:68:A:OP1      | 8:s6:160:ARG:NH2   | 2.30                     | 0.49              |
| 1:6:219:A:H2'     | 1:6:831:U:O2       | 2.13                     | 0.49              |
| 1:6:1657:U:H4'    | 1:6:1658:G:OP2     | 2.13                     | 0.49              |
| 2:s0:93:THR:HG21  | 2:s0:181:VAL:HG21  | 1.95                     | 0.49              |
| 6:s4:29:PRO:O     | 6:s4:30:ARG:HB3    | 2.13                     | 0.49              |
| 9:s7:17:GLU:OE2   | 9:s7:46:ILE:N      | 2.35                     | 0.49              |
| 36:5:378:A:N7     | 36:5:391:A:H2      | 2.11                     | 0.49              |
| 36:5:1192:C:H41   | 36:5:1302:A:P      | 2.35                     | 0.49              |
| 36:5:1631:C:H5''  | 36:5:1632:A:H5''   | 1.94                     | 0.49              |
| 36:5:1875:G:OP2   | 55:m9:20:ARG:HG3   | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:2591:A:O2'    | 36:5:2592:G:H5'    | 2.13                     | 0.49              |
| 36:5:3022:G:O2'    | 36:5:3031:G:O6     | 2.30                     | 0.49              |
| 41:l4:203:ARG:NH1  | 41:l4:226:GLU:OE2  | 2.45                     | 0.49              |
| 42:l5:146:LEU:HD13 | 42:l5:148:ILE:CD1  | 2.42                     | 0.49              |
| 42:l5:273:ARG:O    | 42:l5:273:ARG:HG2  | 2.12                     | 0.49              |
| 50:m4:22:LEU:HB3   | 50:m4:64:VAL:HG13  | 1.95                     | 0.49              |
| 62:n6:39:LEU:HD22  | 62:n6:43:TYR:CE2   | 2.48                     | 0.49              |
| 1:2:325:G:C4'      | 13:C1:80:MET:HE3   | 2.43                     | 0.48              |
| 1:2:1366:U:O2'     | 21:C9:7:ARG:HD2    | 2.12                     | 0.48              |
| 16:C4:12:GLN:HB3   | 16:C4:77:THR:OG1   | 2.12                     | 0.48              |
| 24:D2:110:ILE:HD13 | 24:D2:126:LEU:HD11 | 1.95                     | 0.48              |
| 26:D4:104:SER:HB3  | 26:D4:107:GLN:HG3  | 1.95                     | 0.48              |
| 33:E1:144:CYS:SG   | 33:E1:147:VAL:HG22 | 2.53                     | 0.48              |
| 36:1:900:G:H1'     | 36:1:1589:A:N6     | 2.28                     | 0.48              |
| 36:1:1481:A:OP1    | 36:1:1481:A:O4'    | 2.30                     | 0.48              |
| 36:1:2244:A:H5''   | 39:L2:243:THR:OG1  | 2.12                     | 0.48              |
| 36:1:2319:U:O4     | 86:1:4043:OHX:N2   | 2.46                     | 0.48              |
| 86:1:4023:OHX:N3   | 86:1:4061:OHX:N1   | 2.61                     | 0.48              |
| 86:1:4032:OHX:N4   | 86:1:4149:OHX:N1   | 2.61                     | 0.48              |
| 38:4:79:A:O3'      | 38:4:80:A:H4'      | 2.13                     | 0.48              |
| 41:L4:292:SER:O    | 41:L4:293:SER:OG   | 2.26                     | 0.48              |
| 50:M4:17:VAL:HG22  | 50:M4:36:VAL:O     | 2.12                     | 0.48              |
| 68:O2:126:LEU:O    | 68:O2:128:LEU:N    | 2.44                     | 0.48              |
| 70:O4:22:VAL:HG12  | 70:O4:30:LEU:HD22  | 1.95                     | 0.48              |
| 1:6:542:A:N1       | 80:e0:28:LYS:HD3   | 2.27                     | 0.48              |
| 1:6:1336:A:OP1     | 86:6:2178:OHX:N1   | 2.46                     | 0.48              |
| 2:s0:122:ILE:HG23  | 2:s0:144:ILE:HB    | 1.95                     | 0.48              |
| 3:s1:47:LEU:O      | 16:c4:37:GLU:HG3   | 2.13                     | 0.48              |
| 4:s2:99:LYS:HA     | 4:s2:117:THR:HA    | 1.95                     | 0.48              |
| 10:s8:36:THR:HA    | 10:s8:58:LEU:O     | 2.12                     | 0.48              |
| 11:s9:171:ARG:HH11 | 11:s9:174:ARG:HD3  | 1.76                     | 0.48              |
| 18:c6:93:HIS:HA    | 18:c6:97:VAL:HG23  | 1.95                     | 0.48              |
| 20:c8:101:LEU:O    | 20:c8:104:ASN:HB3  | 2.12                     | 0.48              |
| 36:5:69:C:H2'      | 36:5:70:A:O4'      | 2.13                     | 0.48              |
| 36:5:661:G:P       | 64:n8:12:ARG:HH22  | 2.36                     | 0.48              |
| 36:5:1912:U:N3     | 36:5:2122:G:OP2    | 2.40                     | 0.48              |
| 36:5:2436:U:H3     | 36:5:2511:A:H62    | 1.61                     | 0.48              |
| 40:l3:227:GLU:HG3  | 40:l3:270:ARG:HB3  | 1.95                     | 0.48              |
| 41:l4:232:SER:O    | 41:l4:233:LEU:HB2  | 2.13                     | 0.48              |
| 53:m7:69:ARG:HG2   | 53:m7:79:THR:CG2   | 2.34                     | 0.48              |
| 58:n2:20:SER:O     | 58:n2:24:GLU:HG2   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 60:n4:126:GLU:HG2  | 60:n4:129:LYS:NZ  | 2.27                     | 0.48              |
| 62:n6:59:VAL:HG22  | 62:n6:103:LYS:O   | 2.12                     | 0.48              |
| 64:n8:24:LYS:HD3   | 64:n8:24:LYS:N    | 2.27                     | 0.48              |
| 73:o7:8:PHE:HA     | 73:o7:11:ARG:HD3  | 1.95                     | 0.48              |
| 79:q3:35:ALA:HB3   | 79:q3:37:TYR:CE2  | 2.48                     | 0.48              |
| 1:2:142:G:N2       | 1:2:173:A:C2      | 2.73                     | 0.48              |
| 1:2:213:A:OP2      | 86:2:2116:OHX:N2  | 2.46                     | 0.48              |
| 1:2:1555:A:OP1     | 17:C5:47:ARG:HD3  | 2.12                     | 0.48              |
| 86:2:2076:OHX:N3   | 86:2:2163:OHX:N5  | 2.61                     | 0.48              |
| 5:S3:115:ILE:HG21  | 35:SM:110:TRP:HA  | 1.94                     | 0.48              |
| 8:S6:55:GLY:CA     | 8:S6:63:MET:HE3   | 2.42                     | 0.48              |
| 10:S8:151:LYS:O    | 10:S8:151:LYS:HD3 | 2.13                     | 0.48              |
| 19:C7:66:VAL:HB    | 19:C7:69:ILE:HD11 | 1.95                     | 0.48              |
| 36:1:45:A:OP2      | 51:M5:85:THR:HG21 | 2.13                     | 0.48              |
| 36:1:1170:A:OP2    | 86:1:3962:OHX:N3  | 2.46                     | 0.48              |
| 36:1:2443:A:O2'    | 36:1:2444:C:OP2   | 2.27                     | 0.48              |
| 36:1:2578:U:OP1    | 86:1:4151:OHX:N5  | 2.46                     | 0.48              |
| 36:1:2777:G:H5'    | 36:1:2779:A:OP2   | 2.14                     | 0.48              |
| 36:1:3353:G:O2'    | 36:1:3354:U:OP1   | 2.31                     | 0.48              |
| 41:L4:191:LYS:HG2  | 41:L4:194:TYR:CZ  | 2.48                     | 0.48              |
| 47:M0:86:HIS:HB3   | 47:M0:139:ARG:CG  | 2.43                     | 0.48              |
| 48:M1:9:MET:O      | 48:M1:9:MET:HG3   | 2.13                     | 0.48              |
| 60:N4:86:SER:C     | 60:N4:88:ASP:H    | 2.21                     | 0.48              |
| 65:N9:14:ARG:NH2   | 65:N9:18:ARG:HH11 | 2.09                     | 0.48              |
| 1:6:250:C:H6       | 1:6:250:C:H5'     | 1.78                     | 0.48              |
| 1:6:485:A:C5       | 1:6:486:G:H1'     | 2.48                     | 0.48              |
| 3:s1:77:GLU:OE1    | 16:c4:114:ARG:NH2 | 2.46                     | 0.48              |
| 6:s4:120:SER:O     | 6:s4:164:LEU:HB2  | 2.12                     | 0.48              |
| 11:s9:134:ILE:HD13 | 11:s9:141:VAL:O   | 2.14                     | 0.48              |
| 25:d3:23:ARG:HG3   | 25:d3:23:ARG:NH1  | 2.15                     | 0.48              |
| 36:5:863:C:H2'     | 36:5:864:G:O4'    | 2.13                     | 0.48              |
| 36:5:1003:A:H1'    | 42:l5:15:ARG:CZ   | 2.43                     | 0.48              |
| 36:5:2111:G:H4'    | 36:5:2112:U:OP2   | 2.13                     | 0.48              |
| 36:5:2697:A:H2'    | 36:5:2698:G:C8    | 2.49                     | 0.48              |
| 36:5:2988:C:P      | 52:m6:68:ARG:HH12 | 2.36                     | 0.48              |
| 39:l2:212:GLY:O    | 39:l2:213:GLY:C   | 2.54                     | 0.48              |
| 41:l4:26:PHE:CD1   | 41:l4:130:ALA:HB2 | 2.48                     | 0.48              |
| 45:l8:214:LEU:HD12 | 45:l8:214:LEU:HA  | 1.75                     | 0.48              |
| 47:m0:73:ASN:O     | 47:m0:77:THR:OG1  | 2.20                     | 0.48              |
| 52:m6:72:HIS:O     | 52:m6:74:ARG:HD3  | 2.13                     | 0.48              |
| 63:n7:26:VAL:HG21  | 63:n7:96:VAL:HB   | 1.95                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:n9:24:PRO:HD2   | 65:n9:25:LYS:H     | 1.77                     | 0.48              |
| 69:o3:75:HIS:HB3   | 69:o3:80:VAL:HG12  | 1.94                     | 0.48              |
| 1:2:779:U:OP2      | 1:2:780:A:H2       | 1.96                     | 0.48              |
| 1:2:1236:A:C1'     | 33:E1:138:ARG:HH22 | 2.27                     | 0.48              |
| 14:C2:52:LEU:C     | 14:C2:54:ARG:H     | 2.21                     | 0.48              |
| 29:D7:80:ARG:HG2   | 29:D7:81:ARG:N     | 2.29                     | 0.48              |
| 34:SR:201:THR:HB   | 34:SR:242:SER:HA   | 1.95                     | 0.48              |
| 36:1:357:A:OP2     | 86:O9:101:OHX:N4   | 2.46                     | 0.48              |
| 36:1:591:G:H4'     | 36:1:592:A:OP1     | 2.13                     | 0.48              |
| 36:1:1664:G:H2'    | 36:1:1665:C:C6     | 2.48                     | 0.48              |
| 36:1:1951:C:H5'    | 36:1:1952:G:OP1    | 2.13                     | 0.48              |
| 36:1:2207:A:C2'    | 36:1:2208:A:H5'    | 2.43                     | 0.48              |
| 36:1:2887:A:H2'    | 36:1:2887:A:N3     | 2.27                     | 0.48              |
| 36:1:3166:C:N4     | 36:1:3284:G:H1     | 2.01                     | 0.48              |
| 36:1:3272:C:O2     | 43:L6:80:ASN:HB2   | 2.13                     | 0.48              |
| 37:3:49:G:O6       | 42:L5:58:LYS:NZ    | 2.31                     | 0.48              |
| 40:L3:303:LYS:HD2  | 40:L3:361:THR:HG21 | 1.94                     | 0.48              |
| 41:L4:342:LYS:NZ   | 44:L7:56:GLU:OE2   | 2.25                     | 0.48              |
| 42:L5:114:GLY:C    | 42:L5:116:ASP:N    | 2.72                     | 0.48              |
| 46:L9:13:PRO:HD2   | 46:L9:16:VAL:CG2   | 2.42                     | 0.48              |
| 59:N3:11:PHE:CD1   | 59:N3:88:ARG:HD2   | 2.47                     | 0.48              |
| 78:Q2:3:ASN:HA     | 78:Q2:92:GLU:O     | 2.13                     | 0.48              |
| 1:6:140:A:OP2      | 1:6:140:A:H4'      | 2.13                     | 0.48              |
| 1:6:358:U:O2'      | 1:6:360:A:H5''     | 2.14                     | 0.48              |
| 1:6:737:A:H2'      | 1:6:738:G:H8       | 1.79                     | 0.48              |
| 1:6:753:A:H62      | 6:s4:187:ARG:HH22  | 1.62                     | 0.48              |
| 1:6:1450:U:OP2     | 86:6:2128:OHX:N4   | 2.46                     | 0.48              |
| 1:6:1650:U:H2'     | 1:6:1651:A:C8      | 2.49                     | 0.48              |
| 3:s1:141:ALA:HB1   | 3:s1:207:LEU:HD13  | 1.95                     | 0.48              |
| 5:s3:34:TYR:OH     | 5:s3:37:VAL:HG22   | 2.14                     | 0.48              |
| 5:s3:172:THR:HA    | 5:s3:184:ILE:O     | 2.14                     | 0.48              |
| 10:s8:115:ALA:O    | 10:s8:143:TRP:NE1  | 2.43                     | 0.48              |
| 36:5:585:A:H2'     | 36:5:586:C:C6      | 2.48                     | 0.48              |
| 36:5:847:A:H2'     | 36:5:848:A:C8      | 2.48                     | 0.48              |
| 36:5:3000:A:H2'    | 36:5:3001:C:C6     | 2.48                     | 0.48              |
| 86:5:4076:OHX:N1   | 86:o4:203:OHX:N2   | 2.61                     | 0.48              |
| 39:l2:79:ASN:O     | 39:l2:82:VAL:HG13  | 2.12                     | 0.48              |
| 41:l4:151:VAL:HG12 | 41:l4:152:VAL:H    | 1.78                     | 0.48              |
| 45:l8:165:PHE:HA   | 72:o6:47:ILE:HD13  | 1.95                     | 0.48              |
| 49:m3:2:ALA:N      | 64:n8:33:GLY:O     | 2.46                     | 0.48              |
| 49:m3:106:GLN:HB3  | 72:o6:18:THR:OG1   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:o2:18:LYS:HB3   | 68:o2:30:GLU:HG2   | 1.96                     | 0.48              |
| 68:o2:115:LEU:HB2  | 68:o2:117:ILE:HD12 | 1.93                     | 0.48              |
| 1:2:169:A:OP1      | 8:S6:137:ARG:HG3   | 2.13                     | 0.48              |
| 1:2:190:C:O2'      | 1:2:191:C:H5'      | 2.13                     | 0.48              |
| 1:2:1795:U:O4      | 28:D6:9:GLY:HA2    | 2.13                     | 0.48              |
| 2:S0:69:ASN:HB3    | 2:S0:71:GLU:OE2    | 2.14                     | 0.48              |
| 6:S4:71:LYS:HB2    | 6:S4:75:LYS:O      | 2.14                     | 0.48              |
| 17:C5:21:ASP:OD1   | 17:C5:21:ASP:N     | 2.46                     | 0.48              |
| 17:C5:85:ILE:HD11  | 17:C5:116:LEU:HD23 | 1.94                     | 0.48              |
| 36:1:863:C:OP1     | 86:1:3886:OHX:N5   | 2.46                     | 0.48              |
| 36:1:1231:A:OP2    | 86:1:4089:OHX:N5   | 2.46                     | 0.48              |
| 36:1:1498:A:H2'    | 36:1:1499:C:C6     | 2.48                     | 0.48              |
| 36:1:1672:U:O2'    | 36:1:1673:G:H5'    | 2.13                     | 0.48              |
| 36:1:1798:A:H2'    | 36:1:1799:A:C8     | 2.47                     | 0.48              |
| 36:1:2655:U:H4'    | 36:1:2656:A:O4'    | 2.13                     | 0.48              |
| 36:1:3279:A:C6     | 36:1:3280:U:C4     | 3.02                     | 0.48              |
| 38:4:154:C:H2'     | 38:4:155:A:O4'     | 2.14                     | 0.48              |
| 40:L3:233:TRP:CD1  | 40:L3:265:ALA:HB1  | 2.49                     | 0.48              |
| 47:M0:77:THR:HG22  | 47:M0:85:PHE:HZ    | 1.79                     | 0.48              |
| 63:N7:22:LYS:HD3   | 63:N7:129:TRP:CZ3  | 2.48                     | 0.48              |
| 66:O0:34:LEU:HD23  | 66:O0:59:TYR:HB3   | 1.96                     | 0.48              |
| 71:O5:21:LEU:HD11  | 71:O5:55:LEU:HD21  | 1.95                     | 0.48              |
| 1:6:538:A:H2       | 1:6:540:G:N2       | 2.12                     | 0.48              |
| 1:6:577:G:H3'      | 1:6:577:G:H8       | 1.78                     | 0.48              |
| 1:6:825:U:O2'      | 1:6:826:U:P        | 2.71                     | 0.48              |
| 1:6:1429:G:H21     | 22:d0:72:ASN:ND2   | 2.12                     | 0.48              |
| 1:6:1565:C:OP1     | 20:c8:41:ARG:HD3   | 2.13                     | 0.48              |
| 2:s0:185:ARG:N     | 23:d1:45:ALA:H     | 2.10                     | 0.48              |
| 7:s5:134:VAL:O     | 7:s5:138:THR:HG23  | 2.14                     | 0.48              |
| 19:c7:21:TYR:CD2   | 19:c7:58:MET:HE1   | 2.49                     | 0.48              |
| 19:c7:104:ASN:HA   | 19:c7:107:SER:HB3  | 1.96                     | 0.48              |
| 31:d9:22:ARG:HG2   | 31:d9:37:ASN:O     | 2.14                     | 0.48              |
| 36:5:32:U:O3'      | 51:m5:71:ARG:NH2   | 2.45                     | 0.48              |
| 36:5:1192:C:H5     | 86:5:4091:OHX:N4   | 2.11                     | 0.48              |
| 36:5:2181:C:H5''   | 39:l2:193:ARG:NH2  | 2.28                     | 0.48              |
| 36:5:2209:U:O4     | 86:5:3962:OHX:N4   | 2.46                     | 0.48              |
| 36:5:2655:U:H2'    | 78:q2:3:ASN:O      | 2.14                     | 0.48              |
| 36:5:3157:U:H3'    | 36:5:3158:G:C5'    | 2.43                     | 0.48              |
| 37:7:64:A:H5'      | 37:7:65:G:H5''     | 1.94                     | 0.48              |
| 42:l5:152:ARG:HH11 | 42:l5:152:ARG:CG   | 2.26                     | 0.48              |
| 52:m6:18:ARG:O     | 52:m6:22:VAL:HG13  | 2.13                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:m8:176:ARG:NH1  | 64:n8:46:ASP:OD2   | 2.46                     | 0.48              |
| 63:n7:16:GLY:O     | 63:n7:18:TYR:N     | 2.46                     | 0.48              |
| 73:o7:66:TYR:OH    | 73:o7:73:ARG:NH2   | 2.47                     | 0.48              |
| 77:q1:16:LYS:O     | 77:q1:20:VAL:HG23  | 2.13                     | 0.48              |
| 1:2:219:A:H5'      | 1:2:831:U:O2'      | 2.13                     | 0.48              |
| 1:2:700:C:H42      | 1:2:738:G:H1       | 1.61                     | 0.48              |
| 1:2:850:A:H5'      | 55:M9:165:LYS:HG2  | 1.95                     | 0.48              |
| 1:2:1163:A:N6      | 1:2:1164:G:C6      | 2.81                     | 0.48              |
| 1:2:1435:G:N7      | 12:C0:25:LYS:HE3   | 2.28                     | 0.48              |
| 1:2:1477:G:H2'     | 1:2:1478:G:H8      | 1.76                     | 0.48              |
| 1:2:1642:G:O3'     | 77:Q1:9:ARG:NH2    | 2.46                     | 0.48              |
| 8:S6:119:GLN:HG3   | 8:S6:120:GLU:H     | 1.78                     | 0.48              |
| 20:C8:38:VAL:HG12  | 20:C8:42:TYR:CD2   | 2.48                     | 0.48              |
| 36:1:1080:A:OP2    | 42:L5:140:ARG:NH2  | 2.46                     | 0.48              |
| 36:1:1874:A:H5''   | 55:M9:18:GLY:HA3   | 1.95                     | 0.48              |
| 86:1:3976:OHX:N5   | 86:1:4159:OHX:N1   | 2.62                     | 0.48              |
| 1:6:1318:G:N7      | 86:6:2165:OHX:N5   | 2.61                     | 0.48              |
| 1:6:1590:G:H2'     | 1:6:1591:C:C6      | 2.48                     | 0.48              |
| 1:6:1676:U:H5''    | 10:s8:58:LEU:HD21  | 1.94                     | 0.48              |
| 3:s1:77:GLU:O      | 3:s1:80:SER:OG     | 2.32                     | 0.48              |
| 9:s7:64:VAL:HG22   | 9:s7:94:ALA:HB1    | 1.94                     | 0.48              |
| 10:s8:61:GLU:HG3   | 10:s8:77:ARG:HD2   | 1.96                     | 0.48              |
| 16:c4:122:PRO:C    | 16:c4:124:ASP:H    | 2.22                     | 0.48              |
| 18:c6:115:THR:O    | 18:c6:117:LEU:N    | 2.46                     | 0.48              |
| 22:d0:96:PRO:O     | 22:d0:100:VAL:HG23 | 2.14                     | 0.48              |
| 36:5:904:A:OP2     | 73:o7:30:GLN:NE2   | 2.46                     | 0.48              |
| 86:5:4187:OHX:N1   | 86:5:4189:OHX:N2   | 2.61                     | 0.48              |
| 86:5:4212:OHX:N1   | 86:5:4222:OHX:N5   | 2.60                     | 0.48              |
| 86:7:219:OHX:N3    | 86:7:224:OHX:N6    | 2.61                     | 0.48              |
| 42:l5:41:LYS:HA    | 42:l5:41:LYS:HE3   | 1.94                     | 0.48              |
| 42:l5:45:ASN:O     | 42:l5:47:PRO:HD3   | 2.13                     | 0.48              |
| 51:m5:73:ARG:HG2   | 51:m5:75:VAL:HG22  | 1.94                     | 0.48              |
| 55:m9:163:ARG:HH21 | 55:m9:163:ARG:HG3  | 1.79                     | 0.48              |
| 64:n8:14:HIS:C     | 64:n8:15:VAL:O     | 2.53                     | 0.48              |
| 1:2:248:U:H4'      | 13:C1:36:LYS:HD3   | 1.94                     | 0.48              |
| 1:2:607:G:H5'      | 1:2:613:G:N2       | 2.29                     | 0.48              |
| 1:2:1390:U:O2      | 1:2:1412:G:H1'     | 2.13                     | 0.48              |
| 1:2:1553:G:N2      | 1:2:1555:A:H3'     | 2.29                     | 0.48              |
| 1:2:1625:C:OP1     | 4:S2:91:ARG:NH2    | 2.47                     | 0.48              |
| 86:2:2116:OHX:N5   | 86:C1:201:OHX:N3   | 2.61                     | 0.48              |
| 6:S4:104:ASP:HB3   | 6:S4:105:VAL:H     | 1.44                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:S4:104:ASP:OD2  | 6:S4:108:ARG:HB2   | 2.14                     | 0.48              |
| 14:C2:62:LEU:HA   | 14:C2:120:VAL:HA   | 1.95                     | 0.48              |
| 16:C4:57:PRO:HB3  | 16:C4:100:ALA:HB2  | 1.95                     | 0.48              |
| 19:C7:96:SER:HA   | 19:C7:97:ASN:HA    | 1.52                     | 0.48              |
| 21:C9:25:GLN:HG2  | 21:C9:27:LYS:H     | 1.78                     | 0.48              |
| 21:C9:33:TYR:OH   | 21:C9:103:LYS:HD2  | 2.13                     | 0.48              |
| 36:1:695:C:O2'    | 36:1:696:C:H5'     | 2.13                     | 0.48              |
| 36:1:1932:A:H5'   | 36:1:1933:A:OP2    | 2.13                     | 0.48              |
| 36:1:2094:C:H2'   | 36:1:2095:G:H8     | 1.77                     | 0.48              |
| 36:1:2407:C:H2'   | 36:1:2408:U:C6     | 2.48                     | 0.48              |
| 36:1:2535:A:H3'   | 36:1:2536:A:C8     | 2.49                     | 0.48              |
| 86:1:3973:OHX:N1  | 38:4:31:G:OP2      | 2.46                     | 0.48              |
| 86:1:4059:OHX:N2  | 86:1:4166:OHX:N1   | 2.61                     | 0.48              |
| 39:L2:133:TYR:HB3 | 39:L2:168:VAL:HG12 | 1.95                     | 0.48              |
| 40:L3:256:HIS:HA  | 40:L3:257:PRO:C    | 2.39                     | 0.48              |
| 46:L9:69:ARG:HD3  | 46:L9:72:LYS:HD3   | 1.96                     | 0.48              |
| 47:M0:4:ARG:NH2   | 47:M0:99:ILE:HD12  | 2.29                     | 0.48              |
| 47:M0:36:LEU:HD13 | 47:M0:87:LEU:HD13  | 1.95                     | 0.48              |
| 61:N5:136:ALA:HB1 | 61:N5:141:TYR:CE1  | 2.49                     | 0.48              |
| 74:O8:77:ARG:O    | 74:O8:78:LEU:HB2   | 2.13                     | 0.48              |
| 1:6:517:U:O4      | 86:6:2102:OHX:N4   | 2.47                     | 0.48              |
| 1:6:1050:G:O6     | 86:6:2195:OHX:N4   | 2.46                     | 0.48              |
| 1:6:1417:A:H2'    | 1:6:1418:G:O4'     | 2.14                     | 0.48              |
| 1:6:1489:U:H5'    | 1:6:1494:C:H1'     | 1.95                     | 0.48              |
| 7:s5:192:GLU:OE2  | 27:d5:63:SER:OG    | 2.32                     | 0.48              |
| 8:s6:126:ASP:CG   | 8:s6:127:THR:N     | 2.72                     | 0.48              |
| 8:s6:135:PRO:HB2  | 8:s6:141:ILE:HG12  | 1.96                     | 0.48              |
| 21:c9:6:VAL:HG13  | 21:c9:66:TYR:CZ    | 2.48                     | 0.48              |
| 36:5:1014:U:H3    | 36:5:1036:A:H61    | 1.58                     | 0.48              |
| 36:5:1886:A:O4'   | 36:5:3307:A:H5'    | 2.14                     | 0.48              |
| 36:5:3131:U:H2'   | 36:5:3132:C:C6     | 2.48                     | 0.48              |
| 38:8:26:U:H2'     | 38:8:27:U:C6       | 2.48                     | 0.48              |
| 43:l6:129:GLU:O   | 43:l6:130:ILE:HG12 | 2.13                     | 0.48              |
| 81:m2:23:UNK:O    | 81:m2:28:UNK:N     | 2.46                     | 0.48              |
| 49:m3:42:ARG:HH21 | 49:m3:51:LEU:HD22  | 1.77                     | 0.48              |
| 57:n1:139:ARG:HG2 | 57:n1:139:ARG:NH2  | 2.27                     | 0.48              |
| 66:o0:15:ALA:O    | 66:o0:19:LYS:HG2   | 2.14                     | 0.48              |
| 66:o0:25:LEU:HD22 | 66:o0:90:VAL:HG22  | 1.96                     | 0.48              |
| 66:o0:40:LYS:HD3  | 66:o0:93:LEU:O     | 2.13                     | 0.48              |
| 1:2:263:C:H4'     | 1:2:292:U:H5'      | 1.95                     | 0.48              |
| 1:2:778:G:C8      | 1:2:783:G:C2       | 3.01                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:S0:189:VAL:HG13  | 2:S0:190:ASP:H     | 1.78                     | 0.48              |
| 12:C0:33:GLU:CD    | 12:C0:33:GLU:H     | 2.21                     | 0.48              |
| 16:C4:24:ASN:O     | 16:C4:25:ASP:HB2   | 2.13                     | 0.48              |
| 34:SR:74:THR:HG23  | 34:SR:79:TYR:HB2   | 1.94                     | 0.48              |
| 36:1:1447:G:H3'    | 53:M7:67:ILE:HD11  | 1.95                     | 0.48              |
| 36:1:1506:A:H1'    | 36:1:1848:G:O6     | 2.13                     | 0.48              |
| 36:1:2623:G:C5     | 36:1:2624:G:C5     | 3.01                     | 0.48              |
| 36:1:2713:U:O2'    | 78:Q2:8:ARG:NH1    | 2.47                     | 0.48              |
| 36:1:2897:A:H2'    | 36:1:2899:C:C5'    | 2.43                     | 0.48              |
| 86:1:3980:OHX:N1   | 86:1:4158:OHX:N4   | 2.62                     | 0.48              |
| 86:1:4084:OHX:N4   | 86:1:4153:OHX:N3   | 2.61                     | 0.48              |
| 39:L2:104:LEU:HG   | 39:L2:136:ILE:HD11 | 1.95                     | 0.48              |
| 44:L7:121:LYS:O    | 44:L7:121:LYS:HD3  | 2.13                     | 0.48              |
| 45:L8:101:THR:HG22 | 45:L8:104:GLU:HB2  | 1.96                     | 0.48              |
| 46:L9:12:VAL:HB    | 46:L9:51:GLN:HA    | 1.95                     | 0.48              |
| 50:M4:32:LEU:HD11  | 50:M4:94:TRP:CG    | 2.49                     | 0.48              |
| 63:N7:23:VAL:HG12  | 63:N7:45:GLY:HA3   | 1.95                     | 0.48              |
| 63:N7:47:GLU:CD    | 63:N7:69:LYS:HE2   | 2.39                     | 0.48              |
| 1:6:706:A:H2'      | 1:6:707:A:O4'      | 2.14                     | 0.48              |
| 1:6:1797:A:N1      | 28:d6:87:ARG:HD2   | 2.29                     | 0.48              |
| 2:s0:71:GLU:O      | 2:s0:96:THR:HG22   | 2.13                     | 0.48              |
| 33:e1:103:LEU:HA   | 33:e1:105:TYR:HD2  | 1.79                     | 0.48              |
| 36:5:318:A:OP1     | 86:5:3955:OHX:N5   | 2.46                     | 0.48              |
| 36:5:1408:G:P      | 68:o2:33:ARG:HH22  | 2.36                     | 0.48              |
| 86:5:4201:OHX:N2   | 86:8:224:OHX:N1    | 2.61                     | 0.48              |
| 40:l3:35:ASP:CG    | 40:l3:37:ARG:HD2   | 2.38                     | 0.48              |
| 41:l4:72:ALA:O     | 41:l4:76:ARG:NH1   | 2.47                     | 0.48              |
| 46:l9:49:ASN:OD1   | 46:l9:51:GLN:N     | 2.37                     | 0.48              |
| 51:m5:96:ARG:HG2   | 51:m5:96:ARG:NH1   | 2.28                     | 0.48              |
| 52:m6:121:PRO:HA   | 52:m6:124:LEU:HD22 | 1.95                     | 0.48              |
| 53:m7:128:ARG:HG2  | 53:m7:136:ILE:HG21 | 1.95                     | 0.48              |
| 56:n0:1:MET:HA     | 56:n0:4:PHE:CZ     | 2.49                     | 0.48              |
| 1:2:623:A:OP1      | 86:2:2158:OHX:N4   | 2.47                     | 0.48              |
| 1:2:1115:U:OP1     | 77:Q1:14:LYS:NZ    | 2.43                     | 0.48              |
| 2:S0:74:VAL:HG23   | 2:S0:118:PRO:HB3   | 1.94                     | 0.48              |
| 3:S1:49:ASN:O      | 3:S1:57:ALA:HB2    | 2.14                     | 0.48              |
| 4:S2:58:LEU:HD11   | 4:S2:236:PRO:HG2   | 1.95                     | 0.48              |
| 9:S7:22:GLN:HA     | 9:S7:25:VAL:HG23   | 1.96                     | 0.48              |
| 18:C6:79:TYR:HA    | 18:C6:82:ARG:HD3   | 1.94                     | 0.48              |
| 26:D4:57:VAL:HG13  | 26:D4:60:PHE:HE2   | 1.78                     | 0.48              |
| 36:1:263:C:H2'     | 36:1:264:G:O4'     | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:1157:G:H2'   | 36:1:1158:A:O4'    | 2.14                     | 0.48              |
| 36:1:1260:A:H1'   | 36:1:1280:C:H1'    | 1.95                     | 0.48              |
| 36:1:1547:G:OP1   | 51:M5:105:ARG:HD3  | 2.12                     | 0.48              |
| 36:1:2401:A:O3'   | 41:L4:68:GLY:HA2   | 2.14                     | 0.48              |
| 36:1:3227:A:C2'   | 36:1:3228:C:H5'    | 2.43                     | 0.48              |
| 36:1:3233:C:H2'   | 36:1:3234:A:C8     | 2.49                     | 0.48              |
| 86:1:4036:OHX:N2  | 86:1:4048:OHX:N5   | 2.62                     | 0.48              |
| 86:1:4056:OHX:N2  | 86:1:4163:OHX:N4   | 2.62                     | 0.48              |
| 40:L3:10:ARG:NH2  | 40:L3:14:LEU:HD21  | 2.28                     | 0.48              |
| 40:L3:345:ASN:OD1 | 40:L3:347:SER:HB2  | 2.13                     | 0.48              |
| 43:L6:98:VAL:HA   | 43:L6:101:PHE:CD2  | 2.49                     | 0.48              |
| 46:L9:41:ILE:O    | 46:L9:42:ASP:HB2   | 2.13                     | 0.48              |
| 46:L9:161:LEU:O   | 46:L9:164:ILE:HG22 | 2.13                     | 0.48              |
| 56:N0:132:THR:O   | 56:N0:133:ALA:HB3  | 2.13                     | 0.48              |
| 1:6:93:A:O2'      | 6:s4:4:GLY:HA3     | 2.13                     | 0.48              |
| 1:6:542:A:OP1     | 1:6:544:A:C4       | 2.66                     | 0.48              |
| 1:6:613:G:H4'     | 1:6:614:C:OP1      | 2.13                     | 0.48              |
| 1:6:1392:U:H2'    | 1:6:1393:C:C6      | 2.49                     | 0.48              |
| 1:6:1561:U:H4'    | 1:6:1599:C:H4'     | 1.95                     | 0.48              |
| 1:6:1595:U:N3     | 1:6:1600:A:C2      | 2.72                     | 0.48              |
| 1:6:1793:G:N7     | 28:d6:34:LYS:NZ    | 2.61                     | 0.48              |
| 2:s0:206:ASP:N    | 2:s0:207:PRO:HA    | 2.29                     | 0.48              |
| 7:s5:64:VAL:CG1   | 7:s5:89:ILE:HD11   | 2.44                     | 0.48              |
| 17:c5:110:GLU:H   | 17:c5:110:GLU:CD   | 2.21                     | 0.48              |
| 25:d3:111:GLY:O   | 25:d3:121:ARG:HD2  | 2.13                     | 0.48              |
| 28:d6:90:GLU:H    | 28:d6:90:GLU:CD    | 2.19                     | 0.48              |
| 36:5:314:U:O4     | 86:5:4189:OHX:N5   | 2.46                     | 0.48              |
| 36:5:567:G:H2'    | 36:5:568:G:C8      | 2.48                     | 0.48              |
| 36:5:627:U:H2'    | 36:5:628:A:C8      | 2.49                     | 0.48              |
| 36:5:781:G:OP1    | 54:m8:151:ARG:HD2  | 2.14                     | 0.48              |
| 36:5:1072:G:H2'   | 36:5:1073:U:C6     | 2.48                     | 0.48              |
| 36:5:1081:U:HO2'  | 36:5:1082:U:C5'    | 2.26                     | 0.48              |
| 36:5:1214:U:H2'   | 36:5:1215:U:C6     | 2.48                     | 0.48              |
| 36:5:2355:G:H4'   | 53:m7:139:TYR:CE2  | 2.49                     | 0.48              |
| 36:5:3352:U:O4'   | 36:5:3353:G:C2     | 2.66                     | 0.48              |
| 86:5:4001:OHX:N6  | 86:5:4090:OHX:N5   | 2.62                     | 0.48              |
| 43:l6:40:LEU:HB3  | 43:l6:84:VAL:HG13  | 1.96                     | 0.48              |
| 47:m0:3:ARG:CZ    | 47:m0:63:GLU:HG3   | 2.43                     | 0.48              |
| 48:m1:109:HIS:O   | 48:m1:112:LEU:HD23 | 2.14                     | 0.48              |
| 53:m7:88:VAL:O    | 53:m7:92:GLN:HG3   | 2.13                     | 0.48              |
| 55:m9:35:ALA:O    | 55:m9:36:ASN:ND2   | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:n7:54:THR:HG22  | 63:n7:57:HIS:CE1   | 2.49                     | 0.48              |
| 83:p1:41:UNK:C     | 83:p1:43:UNK:H     | 2.26                     | 0.48              |
| 1:2:97:C:H2'       | 1:2:98:U:C6        | 2.49                     | 0.48              |
| 1:2:397:A:O3'      | 10:S8:50:GLY:HA2   | 2.13                     | 0.48              |
| 1:2:717:C:N4       | 1:2:720:G:H22      | 2.11                     | 0.48              |
| 1:2:939:A:H2'      | 1:2:940:A:C8       | 2.48                     | 0.48              |
| 1:2:1081:A:H2'     | 1:2:1083:G:N7      | 2.29                     | 0.48              |
| 1:2:1370:U:H4'     | 1:2:1371:A:H5'     | 1.96                     | 0.48              |
| 1:2:1570:A:OP1     | 86:2:2155:OHX:N5   | 2.47                     | 0.48              |
| 4:S2:230:TRP:CD2   | 24:D2:68:ARG:HD3   | 2.49                     | 0.48              |
| 7:S5:64:VAL:HG12   | 7:S5:65:ARG:HD3    | 1.95                     | 0.48              |
| 25:D3:13:ARG:O     | 25:D3:17:VAL:HG23  | 2.13                     | 0.48              |
| 36:1:371:G:O6      | 86:1:4183:OHX:N4   | 2.47                     | 0.48              |
| 36:1:690:A:H4'     | 36:1:691:A:OP1     | 2.14                     | 0.48              |
| 36:1:1063:G:N7     | 36:1:1097:G:H2'    | 2.28                     | 0.48              |
| 40:L3:152:LYS:HG3  | 40:L3:192:VAL:HG11 | 1.94                     | 0.48              |
| 44:L7:150:LYS:HD3  | 44:L7:244:ASN:ND2  | 2.28                     | 0.48              |
| 52:M6:23:VAL:O     | 52:M6:27:LEU:HG    | 2.13                     | 0.48              |
| 54:M8:102:ALA:HA   | 54:M8:122:ILE:O    | 2.13                     | 0.48              |
| 54:M8:126:GLN:O    | 54:M8:130:ARG:HG3  | 2.14                     | 0.48              |
| 67:O1:11:GLU:HG2   | 67:O1:74:ARG:HB2   | 1.96                     | 0.48              |
| 1:6:1081:A:O2'     | 1:6:1082:C:O5'     | 2.26                     | 0.48              |
| 1:6:1236:A:H2'     | 1:6:1237:G:C8      | 2.48                     | 0.48              |
| 1:6:1360:A:H3'     | 1:6:1361:U:H4'     | 1.96                     | 0.48              |
| 1:6:1699:G:H22     | 1:6:1702:A:H5''    | 1.78                     | 0.48              |
| 2:s0:92:HIS:HB3    | 2:s0:182:LEU:HD11  | 1.96                     | 0.48              |
| 5:s3:217:ILE:O     | 5:s3:218:LEU:HB2   | 2.13                     | 0.48              |
| 7:s5:59:VAL:O      | 7:s5:61:TYR:N      | 2.46                     | 0.48              |
| 11:s9:171:ARG:CZ   | 11:s9:174:ARG:HD3  | 2.44                     | 0.48              |
| 15:c3:16:ILE:HG13  | 15:c3:62:GLN:HE22  | 1.79                     | 0.48              |
| 16:c4:115:ILE:HG21 | 28:d6:44:ILE:HG21  | 1.95                     | 0.48              |
| 20:c8:83:ALA:HA    | 20:c8:86:LEU:HD22  | 1.95                     | 0.48              |
| 26:d4:15:ASN:HD22  | 26:d4:22:GLN:NE2   | 2.11                     | 0.48              |
| 26:d4:76:TYR:OH    | 26:d4:86:GLU:OE2   | 2.29                     | 0.48              |
| 35:sM:75:ASP:OD1   | 35:sM:75:ASP:N     | 2.37                     | 0.48              |
| 36:5:69:C:OP1      | 51:m5:178:HIS:ND1  | 2.45                     | 0.48              |
| 36:5:75:G:H5''     | 49:m3:58:VAL:HG13  | 1.95                     | 0.48              |
| 36:5:1152:G:OP2    | 36:5:1152:G:H8     | 1.96                     | 0.48              |
| 36:5:1390:A:H5'    | 36:5:1390:A:N3     | 2.29                     | 0.48              |
| 36:5:1614:C:H2'    | 36:5:1615:C:C6     | 2.48                     | 0.48              |
| 86:5:4066:OHX:N3   | 86:5:4141:OHX:N6   | 2.62                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:l3:35:ASP:OD1   | 40:l3:184:ASN:O    | 2.32                     | 0.48              |
| 61:n5:105:VAL:HG11 | 61:n5:126:LEU:HD22 | 1.96                     | 0.48              |
| 82:p0:30:VAL:HG12  | 82:p0:185:LEU:HB2  | 1.95                     | 0.48              |
| 1:2:67:A:C2        | 1:2:69:G:H1'       | 2.49                     | 0.48              |
| 1:2:1160:A:H2'     | 1:2:1161:C:C6      | 2.48                     | 0.48              |
| 86:2:2076:OHX:N4   | 86:2:2163:OHX:N2   | 2.61                     | 0.48              |
| 3:S1:128:LYS:HE3   | 3:S1:132:ASP:HB3   | 1.96                     | 0.48              |
| 3:S1:133:TYR:CG    | 3:S1:181:LEU:HD11  | 2.49                     | 0.48              |
| 4:S2:173:PRO:O     | 4:S2:176:SER:OG    | 2.17                     | 0.48              |
| 5:S3:134:CYS:N     | 5:S3:157:LEU:HD11  | 2.29                     | 0.48              |
| 13:C1:36:LYS:NZ    | 13:C1:59:PRO:O     | 2.43                     | 0.48              |
| 13:C1:94:ILE:HD12  | 25:D3:16:ARG:HD2   | 1.96                     | 0.48              |
| 15:C3:33:VAL:HA    | 15:C3:36:GLN:HB2   | 1.96                     | 0.48              |
| 20:C8:40:ARG:HB3   | 21:C9:45:MET:SD    | 2.54                     | 0.48              |
| 36:1:861:C:H2'     | 36:1:862:U:H6      | 1.78                     | 0.48              |
| 36:1:889:U:H2'     | 36:1:890:C:O4'     | 2.14                     | 0.48              |
| 36:1:1063:G:C6     | 36:1:1097:G:C5     | 3.02                     | 0.48              |
| 36:1:1471:U:H2'    | 36:1:1472:U:C6     | 2.48                     | 0.48              |
| 36:1:2366:C:H5'    | 40:L3:259:HIS:CE1  | 2.49                     | 0.48              |
| 40:L3:53:MET:HE2   | 40:L3:77:THR:HG22  | 1.95                     | 0.48              |
| 42:L5:11:ALA:O     | 42:L5:15:ARG:HG3   | 2.14                     | 0.48              |
| 46:L9:84:LYS:HA    | 46:L9:188:THR:HG23 | 1.96                     | 0.48              |
| 50:M4:84:LYS:O     | 50:M4:87:ALA:HB3   | 2.13                     | 0.48              |
| 55:M9:10:LEU:HD23  | 55:M9:41:ILE:HD13  | 1.96                     | 0.48              |
| 71:O5:85:THR:HB    | 71:O5:88:LEU:HD12  | 1.94                     | 0.48              |
| 6:s4:71:LYS:O      | 6:s4:90:ILE:HA     | 2.13                     | 0.48              |
| 7:s5:64:VAL:HG13   | 7:s5:89:ILE:HD11   | 1.95                     | 0.48              |
| 9:s7:74:GLN:HG2    | 9:s7:131:PHE:HD2   | 1.79                     | 0.48              |
| 16:c4:125:SER:OG   | 16:c4:126:THR:N    | 2.47                     | 0.48              |
| 24:d2:67:GLY:O     | 24:d2:69:LEU:N     | 2.47                     | 0.48              |
| 28:d6:94:ASN:OD1   | 28:d6:96:ALA:HB3   | 2.14                     | 0.48              |
| 29:d7:63:LEU:HD23  | 29:d7:63:LEU:HA    | 1.75                     | 0.48              |
| 36:5:290:G:H4'     | 51:m5:69:GLY:O     | 2.14                     | 0.48              |
| 36:5:415:G:OP2     | 86:5:4219:OHX:N4   | 2.47                     | 0.48              |
| 36:5:595:G:C8      | 36:5:609:G:C6      | 3.02                     | 0.48              |
| 36:5:720:A:O2'     | 36:5:784:A:OP2     | 2.31                     | 0.48              |
| 36:5:1094:U:O2'    | 36:5:1095:U:H3'    | 2.14                     | 0.48              |
| 36:5:2696:A:H2'    | 36:5:2697:A:C8     | 2.49                     | 0.48              |
| 86:5:4094:OHX:N3   | 86:5:4234:OHX:N6   | 2.62                     | 0.48              |
| 37:7:1:G:H21       | 42:l5:269:SER:CB   | 2.27                     | 0.48              |
| 41:l4:326:ARG:O    | 44:l7:41:ARG:NH2   | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:o2:24:ARG:HD3   | 68:o2:25:TYR:CZ    | 2.48                     | 0.48              |
| 74:o8:12:LEU:HD12  | 74:o8:12:LEU:HA    | 1.73                     | 0.48              |
| 82:p0:60:ARG:HG2   | 82:p0:77:LEU:HD22  | 1.96                     | 0.48              |
| 1:2:144:U:H5       | 8:S6:137:ARG:HH12  | 1.62                     | 0.47              |
| 1:2:755:A:H2'      | 1:2:756:A:C8       | 2.49                     | 0.47              |
| 1:2:912:U:H4'      | 1:2:913:G:H2'      | 1.94                     | 0.47              |
| 86:2:2076:OHX:N3   | 86:2:2163:OHX:N1   | 2.62                     | 0.47              |
| 2:S0:10:THR:OG1    | 2:S0:12:GLU:HG2    | 2.13                     | 0.47              |
| 5:S3:107:PHE:O     | 5:S3:111:ASN:HB2   | 2.13                     | 0.47              |
| 7:S5:34:GLN:HG2    | 18:C6:57:LEU:HD13  | 1.95                     | 0.47              |
| 12:C0:48:SER:O     | 12:C0:52:LYS:HG2   | 2.14                     | 0.47              |
| 12:C0:59:PHE:CZ    | 12:C0:62:GLN:HA    | 2.49                     | 0.47              |
| 34:SR:16:HIS:ND1   | 34:SR:39:ASP:OD2   | 2.38                     | 0.47              |
| 36:1:73:C:C2       | 49:M3:59:ARG:HD3   | 2.49                     | 0.47              |
| 36:1:1389:G:OP2    | 86:1:3976:OHX:N4   | 2.47                     | 0.47              |
| 36:1:1863:G:N1     | 36:1:1866:C:OP2    | 2.39                     | 0.47              |
| 36:1:2939:G:OP2    | 40:L3:2:SER:O      | 2.32                     | 0.47              |
| 36:1:3224:G:O6     | 86:1:3897:OHX:N4   | 2.47                     | 0.47              |
| 86:1:3964:OHX:N5   | 86:1:4143:OHX:N3   | 2.62                     | 0.47              |
| 86:1:3976:OHX:N5   | 86:1:4159:OHX:N2   | 2.62                     | 0.47              |
| 40:L3:211:GLN:HE21 | 40:L3:284:ARG:HA   | 1.79                     | 0.47              |
| 42:L5:111:GLN:C    | 42:L5:113:LEU:H    | 2.22                     | 0.47              |
| 46:L9:171:ASP:CG   | 46:L9:173:ARG:HH11 | 2.22                     | 0.47              |
| 49:M3:91:ARG:NH2   | 49:M3:97:VAL:O     | 2.47                     | 0.47              |
| 56:N0:71:LYS:O     | 56:N0:73:LYS:HE2   | 2.14                     | 0.47              |
| 63:N7:46:ILE:HD11  | 63:N7:49:TYR:HA    | 1.96                     | 0.47              |
| 74:O8:9:LYS:NZ     | 74:O8:13:GLU:OE2   | 2.31                     | 0.47              |
| 1:6:1031:U:H4'     | 1:6:1032:G:OP2     | 2.14                     | 0.47              |
| 7:s5:68:ILE:HD13   | 7:s5:69:PHE:N      | 2.29                     | 0.47              |
| 36:5:13:A:H4'      | 61:n5:39:LYS:HG3   | 1.95                     | 0.47              |
| 36:5:1109:U:H2'    | 36:5:1110:U:O4'    | 2.14                     | 0.47              |
| 36:5:1252:A:H2'    | 36:5:1253:U:H5'    | 1.95                     | 0.47              |
| 36:5:2950:G:C5     | 36:5:2979:U:C4     | 3.02                     | 0.47              |
| 36:5:3243:A:C8     | 52:m6:156:LEU:HD13 | 2.49                     | 0.47              |
| 36:5:3357:U:O2'    | 36:5:3358:U:OP1    | 2.32                     | 0.47              |
| 86:5:4201:OHX:N6   | 86:8:224:OHX:N3    | 2.61                     | 0.47              |
| 38:8:67:U:O4       | 86:8:225:OHX:N3    | 2.47                     | 0.47              |
| 39:l2:70:ARG:NH1   | 39:l2:72:ARG:HE    | 2.11                     | 0.47              |
| 40:l3:81:THR:CG2   | 40:l3:81:THR:O     | 2.62                     | 0.47              |
| 48:m1:166:LYS:C    | 48:m1:168:ASP:H    | 2.22                     | 0.47              |
| 56:n0:132:THR:O    | 56:n0:133:ALA:HB3  | 2.12                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 74:o8:5:ILE:HG22  | 74:o8:54:LEU:HD13  | 1.95                     | 0.47              |
| 75:o9:9:ILE:HG22  | 75:o9:13:MET:CE    | 2.44                     | 0.47              |
| 1:2:1157:A:H2'    | 1:2:1160:A:N7      | 2.29                     | 0.47              |
| 1:2:1638:G:P      | 35:SM:94:HIS:HE2   | 2.37                     | 0.47              |
| 86:2:2076:OHX:N6  | 86:2:2163:OHX:N5   | 2.61                     | 0.47              |
| 9:S7:164:TYR:OH   | 9:S7:165:LYS:HE2   | 2.14                     | 0.47              |
| 36:1:38:U:H4'     | 64:N8:32:ARG:HD2   | 1.95                     | 0.47              |
| 86:1:3968:OHX:N5  | 86:1:4076:OHX:N1   | 2.62                     | 0.47              |
| 86:1:4007:OHX:N3  | 86:1:4175:OHX:N1   | 2.62                     | 0.47              |
| 41:L4:226:GLU:OE1 | 41:L4:237:GLN:NE2  | 2.47                     | 0.47              |
| 46:L9:67:ALA:HA   | 46:L9:70:THR:HG23  | 1.96                     | 0.47              |
| 48:M1:54:VAL:HG11 | 48:M1:57:PHE:CD2   | 2.49                     | 0.47              |
| 51:M5:27:VAL:HB   | 51:M5:122:ASN:ND2  | 2.29                     | 0.47              |
| 52:M6:77:SER:HB2  | 52:M6:104:VAL:HG12 | 1.96                     | 0.47              |
| 56:N0:1:MET:O     | 56:N0:2:ALA:HB2    | 2.13                     | 0.47              |
| 64:N8:91:LEU:HD13 | 64:N8:121:VAL:HG21 | 1.95                     | 0.47              |
| 1:6:244:A:OP1     | 6:s4:155:LYS:NZ    | 2.33                     | 0.47              |
| 8:s6:206:ALA:O    | 8:s6:210:GLN:HG3   | 2.14                     | 0.47              |
| 10:s8:140:GLU:HA  | 10:s8:143:TRP:HB2  | 1.97                     | 0.47              |
| 14:c2:88:LEU:O    | 14:c2:89:ILE:HB    | 2.13                     | 0.47              |
| 36:5:36:C:H2'     | 36:5:37:U:H5'      | 1.96                     | 0.47              |
| 36:5:437:G:H8     | 36:5:437:G:OP2     | 1.96                     | 0.47              |
| 36:5:766:U:H4'    | 36:5:767:U:O5'     | 2.13                     | 0.47              |
| 36:5:1571:A:H1'   | 36:5:1572:U:C5     | 2.49                     | 0.47              |
| 45:l8:33:ASN:HD22 | 45:l8:33:ASN:C     | 2.17                     | 0.47              |
| 48:m1:71:VAL:CG1  | 48:m1:75:LYS:HE3   | 2.44                     | 0.47              |
| 52:m6:36:VAL:HB   | 52:m6:108:ILE:HB   | 1.95                     | 0.47              |
| 53:m7:52:LEU:HD13 | 53:m7:88:VAL:HG11  | 1.95                     | 0.47              |
| 66:o0:34:LEU:HD21 | 66:o0:42:ILE:HG21  | 1.96                     | 0.47              |
| 1:2:488:G:H4'     | 1:2:488:G:OP1      | 2.14                     | 0.47              |
| 1:2:600:U:OP2     | 25:D3:108:GLY:HA2  | 2.14                     | 0.47              |
| 1:2:1473:U:O2     | 1:2:1473:U:H2'     | 2.13                     | 0.47              |
| 1:2:1561:U:H2'    | 1:2:1562:G:H8      | 1.80                     | 0.47              |
| 1:2:1727:G:H2'    | 1:2:1728:A:C8      | 2.48                     | 0.47              |
| 2:S0:154:GLU:HA   | 23:D1:63:GLY:HA2   | 1.96                     | 0.47              |
| 2:S0:183:ARG:NH2  | 2:S0:191:ARG:O     | 2.48                     | 0.47              |
| 3:S1:168:ILE:HG12 | 3:S1:197:ILE:HD12  | 1.96                     | 0.47              |
| 7:S5:57:SER:HB3   | 30:D8:53:ILE:HB    | 1.96                     | 0.47              |
| 7:S5:166:ARG:O    | 7:S5:170:GLN:HB2   | 2.14                     | 0.47              |
| 8:S6:68:LEU:HD13  | 8:S6:68:LEU:HA     | 1.63                     | 0.47              |
| 12:C0:14:TYR:CE2  | 12:C0:21:VAL:HG22  | 2.49                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:D0:72:ASN:OD1   | 22:D0:72:ASN:N     | 2.47                     | 0.47              |
| 35:SM:22:PRO:HB3   | 48:M1:38:GLU:OE1   | 2.13                     | 0.47              |
| 36:1:846:A:H2'     | 36:1:847:A:O4'     | 2.14                     | 0.47              |
| 36:1:1110:U:O4     | 86:1:3983:OHX:N5   | 2.47                     | 0.47              |
| 36:1:1345:G:N7     | 86:1:3964:OHX:N4   | 2.62                     | 0.47              |
| 36:1:3118:C:H4'    | 76:Q0:106:ARG:NH2  | 2.23                     | 0.47              |
| 36:1:3218:A:H5''   | 36:1:3219:G:C4     | 2.49                     | 0.47              |
| 86:1:4023:OHX:N6   | 86:1:4061:OHX:N5   | 2.62                     | 0.47              |
| 86:1:4065:OHX:N3   | 86:1:4177:OHX:N1   | 2.62                     | 0.47              |
| 37:3:4:U:H2'       | 37:3:5:G:H8        | 1.75                     | 0.47              |
| 37:3:121:U:H5''    | 42:L5:265:TYR:HE1  | 1.80                     | 0.47              |
| 39:L2:14:SER:OG    | 39:L2:15:ILE:N     | 2.47                     | 0.47              |
| 40:L3:57:VAL:HG23  | 40:L3:358:TRP:HE3  | 1.79                     | 0.47              |
| 42:L5:196:ARG:NH2  | 42:L5:237:GLU:OE2  | 2.47                     | 0.47              |
| 45:L8:108:ARG:O    | 45:L8:112:GLU:HG2  | 2.14                     | 0.47              |
| 1:6:71:A:H2'       | 1:6:72:A:O4'       | 2.15                     | 0.47              |
| 1:6:800:U:H2'      | 1:6:801:G:C8       | 2.47                     | 0.47              |
| 1:6:820:U:H6       | 1:6:820:U:H2'      | 1.36                     | 0.47              |
| 1:6:1230:A:H8      | 1:6:1258:U:C5      | 2.32                     | 0.47              |
| 1:6:1455:G:OP1     | 17:c5:122:THR:HG21 | 2.13                     | 0.47              |
| 1:6:1478:G:H2'     | 1:6:1479:A:O4'     | 2.13                     | 0.47              |
| 6:s4:26:CYS:HB2    | 6:s4:27:TYR:CD2    | 2.50                     | 0.47              |
| 25:d3:100:ASP:OD2  | 25:d3:142:LYS:NZ   | 2.29                     | 0.47              |
| 25:d3:102:VAL:HG12 | 25:d3:127:VAL:HA   | 1.95                     | 0.47              |
| 26:d4:77:ASN:O     | 26:d4:78:SER:HB3   | 2.14                     | 0.47              |
| 27:d5:81:ARG:HH11  | 27:d5:81:ARG:HB2   | 1.79                     | 0.47              |
| 34:sR:260:ILE:HB   | 34:sR:274:LEU:HD12 | 1.96                     | 0.47              |
| 36:5:662:U:OP1     | 64:n8:8:THR:HG21   | 2.14                     | 0.47              |
| 36:5:1329:U:O2'    | 36:5:1330:A:P      | 2.72                     | 0.47              |
| 36:5:3056:U:OP2    | 86:5:3941:OHX:N2   | 2.48                     | 0.47              |
| 49:m3:87:ALA:O     | 49:m3:91:ARG:HG3   | 2.15                     | 0.47              |
| 54:m8:122:ILE:HD11 | 54:m8:130:ARG:CZ   | 2.44                     | 0.47              |
| 56:n0:77:VAL:HG11  | 56:n0:106:LEU:HG   | 1.96                     | 0.47              |
| 68:o2:119:VAL:O    | 68:o2:122:PRO:HD3  | 2.14                     | 0.47              |
| 1:2:373:G:O6       | 86:2:2160:OHX:N6   | 2.48                     | 0.47              |
| 3:S1:36:SER:HB2    | 3:S1:231:LEU:HB3   | 1.96                     | 0.47              |
| 3:S1:149:GLN:HE22  | 3:S1:154:SER:HB2   | 1.77                     | 0.47              |
| 7:S5:123:VAL:O     | 27:D5:58:ARG:HD2   | 2.14                     | 0.47              |
| 11:S9:36:LEU:O     | 32:E0:33:ARG:HG3   | 2.14                     | 0.47              |
| 34:SR:242:SER:O    | 34:SR:292:LEU:HD21 | 2.14                     | 0.47              |
| 36:1:534:U:O2      | 56:N0:146:LYS:HA   | 2.14                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1856:C:H2'    | 36:1:1857:C:H6     | 1.80                     | 0.47              |
| 86:1:4056:OHX:N2   | 86:1:4163:OHX:N1   | 2.62                     | 0.47              |
| 38:4:151:C:C4      | 61:N5:24:LEU:HD11  | 2.50                     | 0.47              |
| 53:M7:64:ASN:HA    | 53:M7:67:ILE:HG12  | 1.97                     | 0.47              |
| 55:M9:101:VAL:HG13 | 55:M9:104:ARG:HH12 | 1.77                     | 0.47              |
| 60:N4:4:GLU:HG2    | 60:N4:30:ARG:HD3   | 1.96                     | 0.47              |
| 1:6:577:G:H3'      | 1:6:577:G:C8       | 2.50                     | 0.47              |
| 1:6:681:U:H4'      | 1:6:682:C:OP1      | 2.14                     | 0.47              |
| 1:6:1253:U:P       | 14:c2:46:ARG:HH12  | 2.37                     | 0.47              |
| 1:6:1542:G:H22     | 1:6:1568:C:H1'     | 1.79                     | 0.47              |
| 6:s4:117:GLU:C     | 6:s4:119:ALA:H     | 2.21                     | 0.47              |
| 16:c4:50:ALA:C     | 16:c4:52:ARG:N     | 2.67                     | 0.47              |
| 17:c5:7:ALA:O      | 17:c5:9:LYS:N      | 2.45                     | 0.47              |
| 25:d3:103:LEU:HB2  | 25:d3:126:LYS:HB2  | 1.95                     | 0.47              |
| 26:d4:40:LEU:O     | 26:d4:44:LEU:HD12  | 2.15                     | 0.47              |
| 36:5:181:U:H1'     | 36:5:236:G:H22     | 1.79                     | 0.47              |
| 36:5:736:A:H2'     | 36:5:737:G:O4'     | 2.15                     | 0.47              |
| 36:5:1018:G:H2'    | 36:5:1019:G:O4'    | 2.15                     | 0.47              |
| 36:5:2298:U:O4     | 36:5:2923:U:H5     | 1.97                     | 0.47              |
| 36:5:2403:G:C2     | 36:5:2404:A:N7     | 2.78                     | 0.47              |
| 36:5:2505:U:H2'    | 36:5:2506:U:C4     | 2.48                     | 0.47              |
| 36:5:2897:A:H2'    | 36:5:2899:C:H5''   | 1.96                     | 0.47              |
| 86:5:4066:OHX:N5   | 86:5:4141:OHX:N6   | 2.62                     | 0.47              |
| 39:l2:206:PRO:HG3  | 39:l2:213:GLY:HA2  | 1.96                     | 0.47              |
| 40:l3:211:GLN:NE2  | 40:l3:283:TYR:O    | 2.46                     | 0.47              |
| 44:l7:96:PRO:O     | 44:l7:100:ARG:HB2  | 2.14                     | 0.47              |
| 53:m7:33:ALA:HB1   | 53:m7:117:ILE:HG12 | 1.97                     | 0.47              |
| 55:m9:52:LYS:O     | 55:m9:52:LYS:HG2   | 2.13                     | 0.47              |
| 55:m9:90:PRO:HG2   | 55:m9:93:VAL:CG2   | 2.44                     | 0.47              |
| 64:n8:128:ARG:HB3  | 72:o6:8:ALA:CB     | 2.44                     | 0.47              |
| 1:2:749:U:H2'      | 1:2:750:U:C6       | 2.49                     | 0.47              |
| 1:2:819:G:N3       | 1:2:820:U:H5       | 2.12                     | 0.47              |
| 1:2:1332:C:O2'     | 5:S3:162:GLN:HB3   | 2.14                     | 0.47              |
| 86:2:2116:OHX:N6   | 86:C1:201:OHX:N3   | 2.63                     | 0.47              |
| 2:S0:73:VAL:O      | 2:S0:95:ALA:HA     | 2.14                     | 0.47              |
| 3:S1:147:ALA:O     | 3:S1:148:ASN:HB3   | 2.13                     | 0.47              |
| 4:S2:139:ILE:CD1   | 4:S2:191:ALA:HB1   | 2.44                     | 0.47              |
| 7:S5:37:GLN:CD     | 18:C6:53:LEU:HD22  | 2.39                     | 0.47              |
| 12:C0:49:LEU:HB3   | 12:C0:55:VAL:CG1   | 2.45                     | 0.47              |
| 17:C5:68:PRO:HG2   | 17:C5:71:GLU:OE2   | 2.14                     | 0.47              |
| 21:C9:117:SER:HB2  | 21:C9:123:ARG:HB2  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:707:U:H2'     | 36:1:708:G:H5''    | 1.96                     | 0.47              |
| 36:1:2535:A:N6     | 36:1:2544:U:H3     | 2.10                     | 0.47              |
| 36:1:2573:G:N7     | 86:1:4002:OHX:N1   | 2.62                     | 0.47              |
| 36:1:2960:C:H2'    | 36:1:2961:G:C8     | 2.49                     | 0.47              |
| 86:1:3873:OHX:N2   | 73:O7:46:SER:OG    | 2.48                     | 0.47              |
| 86:1:4016:OHX:N6   | 70:O4:64:THR:O     | 2.48                     | 0.47              |
| 42:L5:54:ARG:NH2   | 42:L5:147:ASP:OD1  | 2.31                     | 0.47              |
| 61:N5:135:ILE:O    | 61:N5:139:ILE:HG22 | 2.15                     | 0.47              |
| 1:6:916:U:H5''     | 1:6:917:U:OP2      | 2.14                     | 0.47              |
| 1:6:1432:U:H4'     | 1:6:1433:G:H5''    | 1.97                     | 0.47              |
| 1:6:1645:G:H22     | 1:6:1756:A:H2      | 1.60                     | 0.47              |
| 2:s0:139:VAL:CG2   | 4:s2:62:PRO:HG3    | 2.45                     | 0.47              |
| 6:s4:93:ASP:C      | 6:s4:95:THR:H      | 2.23                     | 0.47              |
| 11:s9:145:SER:O    | 11:s9:146:PHE:C    | 2.57                     | 0.47              |
| 11:s9:171:ARG:HE   | 11:s9:174:ARG:CB   | 2.27                     | 0.47              |
| 16:c4:102:LEU:HD11 | 28:d6:45:VAL:HG12  | 1.96                     | 0.47              |
| 20:c8:46:VAL:HG11  | 20:c8:73:MET:HE3   | 1.95                     | 0.47              |
| 34:sR:161:LYS:HE3  | 34:sR:162:ALA:H    | 1.80                     | 0.47              |
| 35:sM:77:THR:C     | 35:sM:79:SER:N     | 2.72                     | 0.47              |
| 36:5:731:U:H2'     | 36:5:732:C:C6      | 2.50                     | 0.47              |
| 36:5:1010:G:N2     | 47:m0:193:ASP:OD1  | 2.48                     | 0.47              |
| 36:5:1818:U:H2'    | 36:5:1819:U:C6     | 2.48                     | 0.47              |
| 36:5:1952:G:H1     | 36:5:2094:C:N4     | 2.09                     | 0.47              |
| 36:5:2749:G:P      | 42:l5:48:LYS:HZ1   | 2.37                     | 0.47              |
| 41:l4:138:ARG:NH2  | 41:l4:240:PRO:HB2  | 2.29                     | 0.47              |
| 44:l7:145:ARG:HA   | 44:l7:185:ILE:HD13 | 1.96                     | 0.47              |
| 45:l8:71:VAL:HG22  | 45:l8:76:ALA:HB2   | 1.96                     | 0.47              |
| 47:m0:24:ARG:HG3   | 47:m0:24:ARG:NH1   | 2.27                     | 0.47              |
| 47:m0:36:LEU:HD12  | 47:m0:87:LEU:HB3   | 1.97                     | 0.47              |
| 52:m6:15:LEU:HD21  | 52:m6:125:ARG:HG3  | 1.96                     | 0.47              |
| 64:n8:66:ALA:HA    | 64:n8:69:TRP:N     | 2.30                     | 0.47              |
| 82:p0:16:ARG:HB2   | 82:p0:66:PHE:CZ    | 2.50                     | 0.47              |
| 1:2:177:U:H1'      | 8:S6:191:ARG:NH1   | 2.29                     | 0.47              |
| 1:2:538:A:H8       | 1:2:543:C:C4       | 2.32                     | 0.47              |
| 1:2:720:G:O2'      | 1:2:721:U:H5'      | 2.15                     | 0.47              |
| 1:2:1175:U:H2'     | 1:2:1176:G:H8      | 1.80                     | 0.47              |
| 1:2:1450:U:H2'     | 1:2:1451:C:H6      | 1.78                     | 0.47              |
| 3:S1:70:LEU:HD21   | 3:S1:79:HIS:CG     | 2.50                     | 0.47              |
| 9:S7:104:ARG:H     | 9:S7:104:ARG:HG2   | 1.35                     | 0.47              |
| 36:1:3281:U:H2'    | 36:1:3282:U:C6     | 2.48                     | 0.47              |
| 36:1:3314:A:OP1    | 40:L3:174:LYS:HB2  | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:L2:40:TYR:HA    | 39:L2:91:GLY:HA3   | 1.97                     | 0.47              |
| 40:L3:56:ILE:HG12  | 40:L3:323:MET:HE1  | 1.96                     | 0.47              |
| 40:L3:152:LYS:HE3  | 40:L3:192:VAL:HG22 | 1.97                     | 0.47              |
| 42:L5:22:ARG:HG2   | 42:L5:28:THR:OG1   | 2.14                     | 0.47              |
| 43:L6:170:LYS:HB3  | 43:L6:172:HIS:CE1  | 2.50                     | 0.47              |
| 46:L9:189:GLU:O    | 46:L9:191:LEU:N    | 2.48                     | 0.47              |
| 52:M6:29:ASN:OD1   | 69:O3:14:LEU:HD22  | 2.15                     | 0.47              |
| 61:N5:113:LEU:HD12 | 61:N5:113:LEU:C    | 2.40                     | 0.47              |
| 63:N7:121:ARG:HG3  | 63:N7:121:ARG:HH11 | 1.80                     | 0.47              |
| 66:O0:16:LEU:HD12  | 66:O0:98:SER:N     | 2.29                     | 0.47              |
| 70:O4:55:SER:OG    | 70:O4:69:HIS:HB3   | 2.13                     | 0.47              |
| 1:6:653:C:N4       | 1:6:677:G:H1       | 2.13                     | 0.47              |
| 1:6:1152:A:OP1     | 28:d6:82:ARG:NH2   | 2.48                     | 0.47              |
| 1:6:1237:G:H2'     | 1:6:1238:A:C8      | 2.49                     | 0.47              |
| 1:6:1255:G:O6      | 14:c2:46:ARG:HD2   | 2.15                     | 0.47              |
| 1:6:1685:G:H1      | 1:6:1716:C:H42     | 1.62                     | 0.47              |
| 1:6:1697:G:H8      | 1:6:1705:C:C2      | 2.32                     | 0.47              |
| 6:s4:62:LYS:HE3    | 6:s4:66:MET:HG2    | 1.95                     | 0.47              |
| 8:s6:63:MET:HE1    | 8:s6:109:LEU:HD23  | 1.95                     | 0.47              |
| 9:s7:89:HIS:CG     | 9:s7:165:LYS:HG2   | 2.50                     | 0.47              |
| 12:c0:22:VAL:HB    | 12:c0:32:HIS:NE2   | 2.29                     | 0.47              |
| 13:c1:101:GLU:CD   | 25:d3:16:ARG:NH2   | 2.72                     | 0.47              |
| 20:c8:88:ARG:NH2   | 20:c8:91:ASP:OD2   | 2.47                     | 0.47              |
| 35:sM:68:ARG:HD2   | 35:sM:68:ARG:C     | 2.39                     | 0.47              |
| 36:5:850:U:H2'     | 36:5:851:C:C6      | 2.50                     | 0.47              |
| 36:5:1949:G:H1     | 36:5:2097:U:H3     | 1.62                     | 0.47              |
| 86:5:3991:OHX:N4   | 38:8:112:U:O2      | 2.48                     | 0.47              |
| 39:l2:77:ILE:CD1   | 39:l2:128:ARG:HB3  | 2.45                     | 0.47              |
| 39:l2:90:ALA:HB2   | 39:l2:101:VAL:HG13 | 1.96                     | 0.47              |
| 42:l5:297:GLN:HG2  | 86:l5:305:OHX:N4   | 2.30                     | 0.47              |
| 47:m0:193:ASP:OD2  | 47:m0:198:LYS:NZ   | 2.46                     | 0.47              |
| 81:m2:143:UNK:O    | 81:m2:145:UNK:N    | 2.47                     | 0.47              |
| 53:m7:136:ILE:O    | 53:m7:137:ASN:ND2  | 2.46                     | 0.47              |
| 1:2:93:A:H1'       | 6:S4:3:ARG:HB3     | 1.97                     | 0.47              |
| 1:2:542:A:H2'      | 1:2:543:C:H3'      | 1.95                     | 0.47              |
| 1:2:720:G:N3       | 1:2:720:G:H2'      | 2.30                     | 0.47              |
| 1:2:894:U:H2'      | 1:2:895:G:H8       | 1.79                     | 0.47              |
| 1:2:900:A:OP1      | 16:C4:43:THR:OG1   | 2.25                     | 0.47              |
| 1:2:912:U:H4'      | 1:2:913:G:O5'      | 2.15                     | 0.47              |
| 1:2:1017:U:H2'     | 1:2:1018:U:C6      | 2.49                     | 0.47              |
| 2:S0:120:LEU:HD12  | 2:S0:121:VAL:H     | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:S1:122:GLU:HG2  | 3:S1:140:ILE:HG13 | 1.97                     | 0.47              |
| 9:S7:116:ARG:HE   | 9:S7:116:ARG:HB2  | 1.57                     | 0.47              |
| 11:S9:122:VAL:O   | 11:S9:125:ALA:HB3 | 2.13                     | 0.47              |
| 21:C9:28:LEU:O    | 21:C9:29:GLU:HB2  | 2.15                     | 0.47              |
| 31:D9:5:ASN:OD1   | 31:D9:7:TRP:NE1   | 2.44                     | 0.47              |
| 31:D9:10:HIS:CG   | 31:D9:11:PRO:HD2  | 2.50                     | 0.47              |
| 36:1:230:U:H2'    | 36:1:231:G:O4'    | 2.13                     | 0.47              |
| 36:1:839:C:H4'    | 36:1:1724:U:H2'   | 1.96                     | 0.47              |
| 36:1:980:A:H2'    | 36:1:981:U:C6     | 2.49                     | 0.47              |
| 36:1:1374:G:O6    | 64:N8:10:LYS:NZ   | 2.47                     | 0.47              |
| 36:1:1815:U:O2'   | 36:1:1816:A:OP2   | 2.28                     | 0.47              |
| 36:1:3227:A:H2'   | 36:1:3228:C:H5'   | 1.95                     | 0.47              |
| 40:L3:339:ARG:HG2 | 40:L3:340:LYS:O   | 2.15                     | 0.47              |
| 41:L4:9:HIS:HE1   | 41:L4:146:PRO:HB2 | 1.78                     | 0.47              |
| 42:L5:257:GLU:O   | 42:L5:258:LYS:HB2 | 2.13                     | 0.47              |
| 43:L6:97:ASN:O    | 43:L6:98:VAL:HB   | 2.15                     | 0.47              |
| 45:L8:67:ILE:HG22 | 45:L8:237:ILE:HB  | 1.96                     | 0.47              |
| 47:M0:86:HIS:ND1  | 47:M0:139:ARG:NH1 | 2.58                     | 0.47              |
| 47:M0:205:SER:O   | 47:M0:209:ASN:HB2 | 2.15                     | 0.47              |
| 49:M3:191:ALA:C   | 49:M3:193:ALA:H   | 2.23                     | 0.47              |
| 54:M8:67:ILE:HG12 | 54:M8:81:VAL:HG21 | 1.97                     | 0.47              |
| 60:N4:22:VAL:HG22 | 60:N4:28:ILE:HG12 | 1.96                     | 0.47              |
| 64:N8:6:THR:CG2   | 64:N8:8:THR:HG23  | 2.39                     | 0.47              |
| 64:N8:103:ASP:OD1 | 64:N8:106:ALA:HB2 | 2.14                     | 0.47              |
| 1:6:654:C:H2'     | 1:6:655:G:C8      | 2.49                     | 0.47              |
| 1:6:898:A:H5''    | 16:c4:46:MET:HE3  | 1.95                     | 0.47              |
| 1:6:1360:A:C4     | 1:6:1361:U:H1'    | 2.50                     | 0.47              |
| 5:s3:64:ARG:NH1   | 5:s3:68:GLU:OE1   | 2.46                     | 0.47              |
| 7:s5:89:ILE:HD12  | 7:s5:90:ILE:N     | 2.29                     | 0.47              |
| 10:s8:70:GLU:OE2  | 10:s8:117:TYR:OH  | 2.24                     | 0.47              |
| 10:s8:115:ALA:O   | 10:s8:117:TYR:N   | 2.48                     | 0.47              |
| 16:c4:99:GLN:NE2  | 28:d6:44:ILE:O    | 2.37                     | 0.47              |
| 16:c4:122:PRO:C   | 16:c4:124:ASP:N   | 2.73                     | 0.47              |
| 20:c8:4:VAL:HG21  | 27:d5:82:HIS:ND1  | 2.29                     | 0.47              |
| 21:c9:33:TYR:O    | 21:c9:35:ASP:N    | 2.44                     | 0.47              |
| 29:d7:19:HIS:CE1  | 29:d7:21:LEU:H    | 2.33                     | 0.47              |
| 29:d7:72:LYS:HB2  | 29:d7:72:LYS:NZ   | 2.30                     | 0.47              |
| 34:sR:79:TYR:HE1  | 34:sR:100:TYR:HE1 | 1.61                     | 0.47              |
| 34:sR:316:MET:C   | 34:sR:318:ALA:H   | 2.22                     | 0.47              |
| 36:5:357:A:OP2    | 86:5:4207:OHX:N5  | 2.47                     | 0.47              |
| 36:5:1369:A:H5''  | 64:n8:21:ARG:HD2  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:5:1915:A:H2'   | 36:5:1916:U:C6    | 2.50                     | 0.47              |
| 36:5:2752:U:O2    | 86:5:4230:OHX:N3  | 2.48                     | 0.47              |
| 36:5:2828:G:OP1   | 47:m0:7:ARG:NH1   | 2.47                     | 0.47              |
| 36:5:2951:G:O2'   | 36:5:2952:G:H5'   | 2.14                     | 0.47              |
| 36:5:3159:C:H2'   | 36:5:3160:U:C6    | 2.50                     | 0.47              |
| 36:5:3160:U:H2'   | 36:5:3161:C:C6    | 2.50                     | 0.47              |
| 36:5:3263:G:O6    | 86:5:4119:OHX:N2  | 2.48                     | 0.47              |
| 86:7:219:OHX:N5   | 86:7:224:OHX:N2   | 2.62                     | 0.47              |
| 38:8:74:U:O2      | 86:8:218:OHX:N5   | 2.47                     | 0.47              |
| 41:l4:271:LYS:HB2 | 41:l4:274:TYR:HB3 | 1.95                     | 0.47              |
| 44:l7:165:ASP:OD2 | 44:l7:166:ASN:N   | 2.48                     | 0.47              |
| 46:l9:85:GLY:O    | 46:l9:186:PHE:HA  | 2.15                     | 0.47              |
| 51:m5:160:GLU:OE1 | 51:m5:160:GLU:N   | 2.46                     | 0.47              |
| 53:m7:30:ARG:HD3  | 53:m7:30:ARG:C    | 2.40                     | 0.47              |
| 62:n6:91:ASN:C    | 62:n6:93:ALA:H    | 2.22                     | 0.47              |
| 65:n9:21:ILE:C    | 65:n9:22:LYS:HZ3  | 2.22                     | 0.47              |
| 73:o7:76:ASN:O    | 73:o7:79:GLN:HG3  | 2.14                     | 0.47              |
| 74:o8:46:ARG:HH21 | 74:o8:51:LEU:HB2  | 1.79                     | 0.47              |
| 1:2:142:G:O5'     | 1:2:142:G:H8      | 1.98                     | 0.47              |
| 1:2:161:U:OP2     | 8:S6:87:ARG:NH2   | 2.48                     | 0.47              |
| 1:2:422:G:OP1     | 86:2:2043:OHX:N6  | 2.48                     | 0.47              |
| 6:S4:159:THR:HG23 | 6:S4:173:ILE:HD13 | 1.97                     | 0.47              |
| 8:S6:63:MET:HE2   | 8:S6:106:LEU:HD22 | 1.96                     | 0.47              |
| 23:D1:39:VAL:HB   | 23:D1:44:ARG:O    | 2.15                     | 0.47              |
| 25:D3:23:ARG:HH11 | 25:D3:23:ARG:HG3  | 1.80                     | 0.47              |
| 36:1:621:A:O2'    | 86:1:4167:OHX:N1  | 2.48                     | 0.47              |
| 36:1:1509:A:H2'   | 36:1:1510:G:C8    | 2.49                     | 0.47              |
| 36:1:1611:G:H2'   | 36:1:1612:A:O4'   | 2.14                     | 0.47              |
| 36:1:2418:G:O6    | 86:1:4122:OHX:N1  | 2.48                     | 0.47              |
| 41:L4:182:LEU:CD1 | 41:L4:223:PRO:HG2 | 2.45                     | 0.47              |
| 41:L4:338:LYS:C   | 41:L4:340:GLY:H   | 2.17                     | 0.47              |
| 45:L8:26:LEU:HD12 | 45:L8:26:LEU:H    | 1.79                     | 0.47              |
| 46:L9:162:GLN:HB2 | 46:L9:179:ILE:O   | 2.15                     | 0.47              |
| 52:M6:116:LYS:HG3 | 52:M6:117:ARG:N   | 2.24                     | 0.47              |
| 73:O7:32:LYS:HD3  | 73:O7:32:LYS:HA   | 1.69                     | 0.47              |
| 1:6:992:A:H5'     | 1:6:992:A:H8      | 1.80                     | 0.47              |
| 1:6:1379:C:H5'    | 18:c6:10:PHE:CE2  | 2.49                     | 0.47              |
| 1:6:1402:G:OP1    | 19:c7:4:VAL:HA    | 2.15                     | 0.47              |
| 1:6:1472:C:H2'    | 1:6:1535:U:O4     | 2.14                     | 0.47              |
| 2:s0:79:ARG:O     | 2:s0:83:GLN:HG3   | 2.15                     | 0.47              |
| 7:s5:222:LYS:HA   | 7:s5:225:ARG:NH1  | 2.26                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:sR:157:VAL:HB  | 34:sR:168:THR:HG22 | 1.96                     | 0.47              |
| 34:sR:205:SER:OG  | 34:sR:207:ASP:OD2  | 2.24                     | 0.47              |
| 36:5:658:G:N2     | 41:l4:93:MET:HB2   | 2.29                     | 0.47              |
| 36:5:1348:U:C6    | 36:5:1355:A:C5     | 3.03                     | 0.47              |
| 36:5:1561:G:H1    | 36:5:1578:C:N4     | 2.12                     | 0.47              |
| 36:5:2209:U:H4'   | 36:5:2210:G:OP1    | 2.14                     | 0.47              |
| 86:5:4023:OHX:N4  | 86:5:4215:OHX:N3   | 2.63                     | 0.47              |
| 38:8:141:C:OP1    | 51:m5:109:ARG:NH1  | 2.47                     | 0.47              |
| 39:l2:204:MET:HE3 | 39:l2:208:ASP:CB   | 2.44                     | 0.47              |
| 47:m0:74:LYS:O    | 47:m0:78:THR:HG23  | 2.15                     | 0.47              |
| 56:n0:12:ARG:HD2  | 56:n0:22:PRO:HG2   | 1.96                     | 0.47              |
| 58:n2:54:VAL:HG13 | 58:n2:67:SER:HB2   | 1.97                     | 0.47              |
| 64:n8:84:GLU:O    | 64:n8:87:ARG:HB2   | 2.14                     | 0.47              |
| 67:o1:25:PHE:HB3  | 67:o1:65:LYS:HG3   | 1.96                     | 0.47              |
| 71:o5:59:ASN:O    | 71:o5:63:ARG:HG2   | 2.15                     | 0.47              |
| 1:2:1789:G:OP2    | 16:C4:132:ARG:NH2  | 2.41                     | 0.47              |
| 86:2:2045:OHX:N4  | 86:2:2099:OHX:N6   | 2.63                     | 0.47              |
| 2:S0:71:GLU:HA    | 2:S0:95:ALA:N      | 2.30                     | 0.47              |
| 2:S0:101:ARG:HG3  | 2:S0:102:PHE:N     | 2.29                     | 0.47              |
| 3:S1:63:GLY:HA2   | 3:S1:88:VAL:O      | 2.14                     | 0.47              |
| 7:S5:103:ASN:HA   | 7:S5:106:LYS:HD2   | 1.97                     | 0.47              |
| 17:C5:69:GLU:OE1  | 86:C5:201:OHX:N2   | 2.48                     | 0.47              |
| 19:C7:24:LEU:HD13 | 19:C7:58:MET:HE3   | 1.96                     | 0.47              |
| 20:C8:35:ILE:HB   | 20:C8:38:VAL:CG2   | 2.45                     | 0.47              |
| 21:C9:126:GLU:H   | 21:C9:126:GLU:CD   | 2.23                     | 0.47              |
| 36:1:1926:C:H5'   | 36:1:1927:G:C5     | 2.49                     | 0.47              |
| 86:1:3968:OHX:N6  | 86:1:4076:OHX:N2   | 2.63                     | 0.47              |
| 37:3:19:C:H2'     | 37:3:20:A:H8       | 1.79                     | 0.47              |
| 38:4:26:U:H2'     | 38:4:27:U:C6       | 2.50                     | 0.47              |
| 44:L7:137:GLY:HA3 | 44:L7:236:ILE:HB   | 1.96                     | 0.47              |
| 74:O8:17:ARG:O    | 74:O8:19:ASP:N     | 2.41                     | 0.47              |
| 76:Q0:93:LYS:HB3  | 76:Q0:103:LEU:O    | 2.15                     | 0.47              |
| 1:6:652:G:N2      | 1:6:683:C:C2       | 2.82                     | 0.47              |
| 2:s0:125:ASP:HB3  | 2:s0:128:SER:HB2   | 1.95                     | 0.47              |
| 2:s0:167:LYS:HB3  | 2:s0:168:HIS:H     | 1.20                     | 0.47              |
| 3:s1:30:PHE:HB3   | 3:s1:96:LEU:HD22   | 1.96                     | 0.47              |
| 4:s2:53:ILE:HG12  | 4:s2:73:LEU:HD22   | 1.97                     | 0.47              |
| 7:s5:109:LYS:O    | 7:s5:113:ILE:HG13  | 2.15                     | 0.47              |
| 7:s5:167:ARG:HH21 | 30:d8:55:VAL:HG21  | 1.79                     | 0.47              |
| 11:s9:121:SER:HB3 | 11:s9:124:HIS:H    | 1.80                     | 0.47              |
| 13:c1:108:PRO:HG2 | 13:c1:134:THR:O    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:e0:39:LEU:O     | 80:e0:43:ARG:HB2   | 2.15                     | 0.47              |
| 36:5:701:G:H2'     | 36:5:702:C:C6      | 2.49                     | 0.47              |
| 36:5:1049:C:H2'    | 36:5:1050:U:C6     | 2.50                     | 0.47              |
| 36:5:1213:G:OP1    | 56:n0:137:ARG:HD3  | 2.15                     | 0.47              |
| 36:5:1438:U:H2'    | 36:5:1439:U:C6     | 2.49                     | 0.47              |
| 36:5:2836:C:O2     | 36:5:2836:C:O4'    | 2.28                     | 0.47              |
| 37:7:98:C:OP1      | 56:n0:39:SER:OG    | 2.27                     | 0.47              |
| 38:8:38:U:O4       | 71:o5:89:ARG:HD2   | 2.15                     | 0.47              |
| 39:l2:30:ARG:NH2   | 39:l2:33:ASP:OD2   | 2.48                     | 0.47              |
| 39:l2:55:GLY:O     | 39:l2:56:ALA:HB3   | 2.15                     | 0.47              |
| 40:l3:53:MET:HE2   | 40:l3:77:THR:CG2   | 2.45                     | 0.47              |
| 81:m2:63:UNK:HA    | 81:m2:71:UNK:O     | 2.15                     | 0.47              |
| 49:m3:82:ALA:C     | 49:m3:84:GLY:H     | 2.22                     | 0.47              |
| 49:m3:162:ASN:HD21 | 49:m3:164:GLU:HB2  | 1.80                     | 0.47              |
| 63:n7:4:PHE:O      | 63:n7:5:LEU:HB2    | 2.13                     | 0.47              |
| 63:n7:15:ARG:HD2   | 63:n7:79:HIS:CD2   | 2.50                     | 0.47              |
| 65:n9:9:ALA:O      | 65:n9:10:HIS:C     | 2.58                     | 0.47              |
| 74:o8:62:ALA:C     | 74:o8:64:LYS:H     | 2.22                     | 0.47              |
| 79:q3:84:ARG:O     | 79:q3:88:GLU:HG3   | 2.15                     | 0.47              |
| 82:p0:69:ASP:HB2   | 82:p0:70:LEU:HD23  | 1.96                     | 0.47              |
| 1:2:717:C:H2'      | 1:2:718:U:H5''     | 1.98                     | 0.47              |
| 1:2:927:C:H1'      | 16:C4:125:SER:CB   | 2.45                     | 0.47              |
| 1:2:1029:U:O4      | 86:2:2170:OHX:N3   | 2.48                     | 0.47              |
| 1:2:1274:C:C5      | 35:SM:95:SER:HA    | 2.50                     | 0.47              |
| 1:2:1424:A:H1'     | 4:S2:92:ALA:HB1    | 1.97                     | 0.47              |
| 1:2:1762:A:C1'     | 1:2:1783:C:H5'     | 2.45                     | 0.47              |
| 86:2:2096:OHX:N3   | 86:2:2109:OHX:N1   | 2.62                     | 0.47              |
| 6:S4:37:LYS:HB2    | 6:S4:40:GLU:HG2    | 1.97                     | 0.47              |
| 6:S4:212:ASP:OD1   | 6:S4:214:LEU:N     | 2.48                     | 0.47              |
| 7:S5:100:ASN:O     | 7:S5:102:ARG:N     | 2.47                     | 0.47              |
| 7:S5:133:VAL:HG22  | 7:S5:198:LEU:HD13  | 1.97                     | 0.47              |
| 11:S9:108:ARG:HG2  | 11:S9:147:MET:HE2  | 1.95                     | 0.47              |
| 16:C4:81:VAL:HG22  | 16:C4:115:ILE:HB   | 1.97                     | 0.47              |
| 36:1:191:U:H6      | 36:1:191:U:H5'     | 1.79                     | 0.47              |
| 36:1:1227:C:H5'    | 36:1:1228:C:OP2    | 2.15                     | 0.47              |
| 36:1:1645:U:C2'    | 36:1:1646:G:H5'    | 2.45                     | 0.47              |
| 36:1:1674:G:OP2    | 86:1:3952:OHX:N2   | 2.48                     | 0.47              |
| 36:1:2404:A:H2'    | 36:1:2404:A:N3     | 2.30                     | 0.47              |
| 39:L2:202:VAL:HG23 | 39:L2:211:HIS:HB3  | 1.96                     | 0.47              |
| 51:M5:102:ALA:O    | 51:M5:106:VAL:HG13 | 2.15                     | 0.47              |
| 54:M8:64:VAL:O     | 54:M8:96:PHE:HE2   | 1.98                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:M8:123:THR:OG1  | 54:M8:125:ASP:OD2  | 2.24                     | 0.47              |
| 58:N2:58:GLU:C     | 58:N2:60:GLY:H     | 2.21                     | 0.47              |
| 59:N3:13:ILE:CG2   | 59:N3:85:TRP:CD1   | 2.98                     | 0.47              |
| 59:N3:80:ARG:HH12  | 59:N3:116:GLY:HA3  | 1.79                     | 0.47              |
| 66:O0:73:GLY:O     | 66:O0:76:GLU:HG2   | 2.15                     | 0.47              |
| 79:Q3:3:LYS:HB3    | 79:Q3:3:LYS:HE2    | 1.57                     | 0.47              |
| 1:6:76:A:H3'       | 86:6:2192:OHX:N1   | 2.30                     | 0.47              |
| 1:6:1241:G:H2'     | 1:6:1242:A:O4'     | 2.14                     | 0.47              |
| 1:6:1460:A:OP1     | 35:sM:68:ARG:HG2   | 2.14                     | 0.47              |
| 1:6:1503:A:H2'     | 1:6:1504:G:O4'     | 2.14                     | 0.47              |
| 4:s2:59:HIS:CE1    | 4:s2:238:SER:HA    | 2.49                     | 0.47              |
| 7:s5:43:PHE:CZ     | 7:s5:90:ILE:HG21   | 2.50                     | 0.47              |
| 9:s7:39:ARG:NH2    | 55:m9:185:LEU:HD22 | 2.29                     | 0.47              |
| 24:d2:11:LEU:O     | 24:d2:15:ASN:HB2   | 2.15                     | 0.47              |
| 27:d5:85:LYS:HG3   | 27:d5:86:GLU:N     | 2.30                     | 0.47              |
| 35:sM:43:ASP:OD1   | 35:sM:45:SER:OG    | 2.21                     | 0.47              |
| 36:5:817:A:C4      | 73:o7:13:ASN:O     | 2.68                     | 0.47              |
| 36:5:926:A:H2'     | 36:5:927:C:H6      | 1.80                     | 0.47              |
| 36:5:1013:G:H2'    | 36:5:1014:U:O4'    | 2.16                     | 0.47              |
| 36:5:1313:G:H5'    | 52:m6:83:ALA:CB    | 2.45                     | 0.47              |
| 36:5:1728:G:O2'    | 66:o0:87:VAL:HB    | 2.15                     | 0.47              |
| 36:5:2960:C:H2'    | 36:5:2961:G:C8     | 2.50                     | 0.47              |
| 38:8:73:U:OP1      | 62:n6:24:SER:OG    | 2.26                     | 0.47              |
| 42:l5:99:TYR:CD2   | 42:l5:199:ILE:HG12 | 2.50                     | 0.47              |
| 42:l5:155:THR:HG22 | 42:l5:179:ARG:HH11 | 1.80                     | 0.47              |
| 45:l8:105:LYS:HG3  | 45:l8:109:LEU:HD23 | 1.97                     | 0.47              |
| 47:m0:36:LEU:CD1   | 47:m0:87:LEU:HB3   | 2.44                     | 0.47              |
| 47:m0:156:ARG:HG2  | 47:m0:163:GLN:CG   | 2.44                     | 0.47              |
| 55:m9:142:ILE:O    | 55:m9:146:LYS:HG2  | 2.14                     | 0.47              |
| 67:o1:13:THR:CG2   | 67:o1:72:ARG:HH21  | 2.28                     | 0.47              |
| 72:o6:9:ILE:HA     | 72:o6:13:LYS:HD3   | 1.97                     | 0.47              |
| 79:q3:75:ALA:HA    | 79:q3:78:THR:HG23  | 1.96                     | 0.47              |
| 1:2:320:U:H2'      | 1:2:321:C:C6       | 2.51                     | 0.46              |
| 1:2:1217:A:H5'     | 1:2:1217:A:C8      | 2.49                     | 0.46              |
| 1:2:1389:C:O2'     | 19:C7:52:GLY:HA3   | 2.15                     | 0.46              |
| 1:2:1746:A:H2'     | 1:2:1747:G:O4'     | 2.15                     | 0.46              |
| 1:2:1762:A:H1'     | 1:2:1783:C:H5'     | 1.97                     | 0.46              |
| 5:S3:21:LEU:HD22   | 5:S3:25:PHE:CE2    | 2.50                     | 0.46              |
| 6:S4:54:TYR:OH     | 6:S4:97:GLU:OE2    | 2.30                     | 0.46              |
| 8:S6:56:ASN:ND2    | 8:S6:60:GLY:O      | 2.49                     | 0.46              |
| 9:S7:185:ILE:HG22  | 9:S7:186:PRO:HD2   | 1.97                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:C5:18:ARG:HG2   | 20:C8:92:ILE:HA   | 1.95                     | 0.46              |
| 25:D3:54:LEU:HD11  | 25:D3:75:GLN:HB2  | 1.97                     | 0.46              |
| 25:D3:88:PRO:O     | 25:D3:89:ASN:HB2  | 2.15                     | 0.46              |
| 36:1:2186:U:OP2    | 39:L2:200:ARG:HD2 | 2.14                     | 0.46              |
| 36:1:2419:A:H2'    | 36:1:2420:C:C6    | 2.50                     | 0.46              |
| 36:1:3187:A:H5''   | 50:M4:8:LYS:HD2   | 1.96                     | 0.46              |
| 86:1:4071:OHX:N5   | 86:1:4118:OHX:N2  | 2.63                     | 0.46              |
| 46:L9:7:GLU:CD     | 46:L9:54:LYS:HE3  | 2.40                     | 0.46              |
| 64:N8:29:PRO:O     | 64:N8:31:GLY:N    | 2.48                     | 0.46              |
| 1:6:399:A:N3       | 6:s4:3:ARG:NH1    | 2.63                     | 0.46              |
| 1:6:470:A:OP2      | 86:6:2103:OHX:N1  | 2.48                     | 0.46              |
| 1:6:1341:A:OP1     | 34:sR:63:GLY:HA2  | 2.15                     | 0.46              |
| 3:s1:23:PRO:O      | 3:s1:26:ARG:HB3   | 2.14                     | 0.46              |
| 3:s1:70:LEU:HD13   | 3:s1:79:HIS:CG    | 2.50                     | 0.46              |
| 11:s9:171:ARG:HA   | 11:s9:174:ARG:HB2 | 1.97                     | 0.46              |
| 14:c2:67:THR:C     | 14:c2:69:ALA:H    | 2.22                     | 0.46              |
| 20:c8:5:VAL:O      | 27:d5:42:LEU:HB2  | 2.15                     | 0.46              |
| 35:sM:34:LYS:HD3   | 35:sM:34:LYS:HA   | 1.58                     | 0.46              |
| 36:5:239:G:N7      | 86:5:4131:OHX:N5  | 2.63                     | 0.46              |
| 36:5:508:U:H2'     | 36:5:509:U:C6     | 2.50                     | 0.46              |
| 36:5:1016:C:C6     | 36:5:1016:C:OP1   | 2.68                     | 0.46              |
| 36:5:1307:G:H5''   | 52:m6:60:LYS:CE   | 2.44                     | 0.46              |
| 36:5:1310:G:N7     | 86:5:4026:OHX:N4  | 2.62                     | 0.46              |
| 36:5:2541:U:H4'    | 36:5:2542:U:OP1   | 2.16                     | 0.46              |
| 86:5:3973:OHX:N1   | 86:5:4241:OHX:N1  | 2.63                     | 0.46              |
| 40:l3:169:THR:HG23 | 40:l3:171:LEU:HG  | 1.97                     | 0.46              |
| 81:m2:34:UNK:O     | 81:m2:36:UNK:N    | 2.48                     | 0.46              |
| 64:n8:27:LYS:HE2   | 64:n8:27:LYS:HB3  | 1.69                     | 0.46              |
| 64:n8:45:MET:HE2   | 64:n8:45:MET:HA   | 1.97                     | 0.46              |
| 67:o1:13:THR:HG22  | 67:o1:72:ARG:CD   | 2.45                     | 0.46              |
| 67:o1:34:LYS:HE2   | 67:o1:34:LYS:HB2  | 1.68                     | 0.46              |
| 73:o7:2:GLY:O      | 73:o7:7:SER:HB3   | 2.15                     | 0.46              |
| 1:2:1498:G:H5''    | 21:C9:72:GLY:HA3  | 1.97                     | 0.46              |
| 1:2:1507:G:O6      | 86:2:2147:OHX:N5  | 2.48                     | 0.46              |
| 7:S5:126:ASP:HB3   | 7:S5:127:GLN:H    | 1.50                     | 0.46              |
| 11:S9:38:ASN:HB3   | 11:S9:40:LYS:H    | 1.80                     | 0.46              |
| 23:D1:1:MET:O      | 23:D1:9:VAL:HG12  | 2.15                     | 0.46              |
| 24:D2:28:ARG:HA    | 24:D2:29:PRO:HA   | 1.66                     | 0.46              |
| 24:D2:80:ASN:OD1   | 24:D2:124:LYS:HG2 | 2.15                     | 0.46              |
| 34:SR:205:SER:HB3  | 34:SR:210:LEU:HB2 | 1.97                     | 0.46              |
| 36:1:59:G:H2'      | 38:4:33:A:O2'     | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:1:1245:A:C3'    | 36:1:1246:G:H5''  | 2.46                     | 0.46              |
| 86:1:4088:OHX:N2   | 86:1:4157:OHX:N4  | 2.62                     | 0.46              |
| 39:L2:192:LYS:HB3  | 39:L2:193:ARG:NH2 | 2.30                     | 0.46              |
| 40:L3:230:THR:OG1  | 40:L3:247:ARG:HB3 | 2.14                     | 0.46              |
| 66:O0:86:ARG:NH1   | 79:Q3:44:LYS:HG2  | 2.31                     | 0.46              |
| 70:O4:81:CYS:O     | 70:O4:82:ALA:HB3  | 2.15                     | 0.46              |
| 72:O6:33:ALA:O     | 72:O6:34:SER:HB3  | 2.16                     | 0.46              |
| 79:Q3:50:GLY:O     | 79:Q3:51:ALA:HB3  | 2.15                     | 0.46              |
| 1:6:188:A:H2'      | 1:6:189:C:O4'     | 2.15                     | 0.46              |
| 1:6:276:C:H1'      | 1:6:277:U:H5      | 1.80                     | 0.46              |
| 1:6:872:G:H2'      | 1:6:873:U:O4'     | 2.14                     | 0.46              |
| 1:6:1045:C:C2      | 1:6:1074:G:C2     | 3.02                     | 0.46              |
| 20:c8:145:ARG:HA   | 20:c8:145:ARG:HE  | 1.79                     | 0.46              |
| 22:d0:97:VAL:HG13  | 22:d0:98:GLN:H    | 1.80                     | 0.46              |
| 34:sR:13:LEU:HB3   | 34:sR:45:TRP:CZ3  | 2.51                     | 0.46              |
| 36:5:741:U:H2'     | 36:5:742:G:O4'    | 2.15                     | 0.46              |
| 36:5:1295:G:OP1    | 56:n0:84:ARG:HG3  | 2.16                     | 0.46              |
| 36:5:1517:G:P      | 75:o9:41:ARG:HH22 | 2.39                     | 0.46              |
| 36:5:3358:U:H2'    | 36:5:3359:A:H8    | 1.81                     | 0.46              |
| 86:5:3921:OHX:N4   | 51:m5:91:GLU:OE2  | 2.47                     | 0.46              |
| 86:5:4001:OHX:N3   | 86:5:4090:OHX:N5  | 2.63                     | 0.46              |
| 40:l3:221:THR:HG22 | 40:l3:272:TYR:N   | 2.30                     | 0.46              |
| 41:l4:84:ARG:O     | 41:l4:87:GLN:HG3  | 2.16                     | 0.46              |
| 43:l6:51:ARG:NH1   | 50:m4:114:ASP:OD2 | 2.48                     | 0.46              |
| 43:l6:68:PRO:HG2   | 43:l6:71:VAL:CG2  | 2.44                     | 0.46              |
| 52:m6:42:ASN:OD1   | 52:m6:125:ARG:HD3 | 2.15                     | 0.46              |
| 1:2:356:G:OP2      | 86:2:2037:OHX:N6  | 2.48                     | 0.46              |
| 1:2:702:G:C6       | 1:2:737:A:C6      | 3.03                     | 0.46              |
| 1:2:1560:U:O2      | 1:2:1560:U:O4'    | 2.31                     | 0.46              |
| 1:2:1595:U:H5      | 1:2:1596:C:C5     | 2.34                     | 0.46              |
| 1:2:1759:C:O2'     | 36:1:2263:C:H4'   | 2.15                     | 0.46              |
| 86:2:2096:OHX:N6   | 86:2:2109:OHX:N5  | 2.63                     | 0.46              |
| 2:S0:169:SER:O     | 2:S0:173:ILE:HG12 | 2.15                     | 0.46              |
| 11:S9:53:ARG:O     | 11:S9:57:ARG:HG3  | 2.15                     | 0.46              |
| 16:C4:124:ASP:O    | 16:C4:125:SER:HB2 | 2.15                     | 0.46              |
| 25:D3:86:PHE:O     | 25:D3:88:PRO:HD3  | 2.16                     | 0.46              |
| 26:D4:27:VAL:HG11  | 26:D4:35:VAL:HG11 | 1.97                     | 0.46              |
| 26:D4:53:ASP:CG    | 26:D4:96:LEU:HD21 | 2.40                     | 0.46              |
| 36:1:1433:A:P      | 68:O2:19:ARG:HH22 | 2.38                     | 0.46              |
| 36:1:1811:G:H2'    | 36:1:1812:G:O4'   | 2.15                     | 0.46              |
| 36:1:2683:U:H2'    | 36:1:2684:C:H6    | 1.80                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:M0:145:LYS:NZ   | 47:M0:167:LEU:HD11 | 2.31                     | 0.46              |
| 51:M5:109:ARG:HA   | 51:M5:109:ARG:HD3  | 1.77                     | 0.46              |
| 57:N1:160:ILE:HD12 | 57:N1:160:ILE:HA   | 1.72                     | 0.46              |
| 86:6:2150:OHX:N4   | 86:c1:202:OHX:N2   | 2.63                     | 0.46              |
| 5:s3:29:LEU:HD21   | 5:s3:69:LEU:HD21   | 1.97                     | 0.46              |
| 7:s5:73:THR:HG23   | 18:c6:114:ARG:HB3  | 1.96                     | 0.46              |
| 12:c0:23:ALA:O     | 12:c0:24:LYS:HB3   | 2.14                     | 0.46              |
| 17:c5:119:PHE:HA   | 35:sM:57:ASN:ND2   | 2.31                     | 0.46              |
| 20:c8:27:LYS:O     | 20:c8:31:ALA:N     | 2.39                     | 0.46              |
| 20:c8:87:ASN:OD1   | 20:c8:99:HIS:HA    | 2.15                     | 0.46              |
| 21:c9:45:MET:HE3   | 21:c9:46:PRO:HD2   | 1.96                     | 0.46              |
| 36:5:2403:G:H5'    | 36:5:2871:G:H5'    | 1.96                     | 0.46              |
| 40:l3:105:VAL:HG21 | 40:l3:148:LEU:HD13 | 1.97                     | 0.46              |
| 71:o5:101:THR:CG2  | 71:o5:104:GLN:H    | 2.21                     | 0.46              |
| 1:2:799:A:H5''     | 6:S4:201:HIS:CD2   | 2.50                     | 0.46              |
| 1:2:1051:G:O2'     | 1:2:1052:U:P       | 2.73                     | 0.46              |
| 1:2:1252:C:O4'     | 33:E1:133:ALA:HB2  | 2.14                     | 0.46              |
| 7:S5:95:ASN:O      | 7:S5:98:MET:HG2    | 2.14                     | 0.46              |
| 7:S5:145:ASP:CG    | 7:S5:146:THR:H     | 2.23                     | 0.46              |
| 14:C2:52:LEU:HA    | 14:C2:85:LYS:HZ1   | 1.80                     | 0.46              |
| 25:D3:62:LYS:HD2   | 25:D3:118:PRO:HB3  | 1.98                     | 0.46              |
| 29:D7:63:LEU:O     | 29:D7:74:SER:N     | 2.44                     | 0.46              |
| 36:1:99:A:H5''     | 51:M5:194:GLN:OE1  | 2.16                     | 0.46              |
| 36:1:2104:A:OP2    | 55:M9:81:ARG:NH2   | 2.39                     | 0.46              |
| 36:1:2426:U:H2'    | 36:1:2427:U:C6     | 2.51                     | 0.46              |
| 86:1:4007:OHX:N4   | 86:1:4175:OHX:N1   | 2.62                     | 0.46              |
| 39:L2:80:GLU:HG3   | 79:Q3:66:GLY:HA2   | 1.97                     | 0.46              |
| 42:L5:68:THR:HG22  | 42:L5:70:THR:H     | 1.80                     | 0.46              |
| 47:M0:47:PRO:HB3   | 47:M0:171:TRP:CE2  | 2.50                     | 0.46              |
| 48:M1:47:GLN:HG2   | 48:M1:67:VAL:HG12  | 1.97                     | 0.46              |
| 50:M4:55:ARG:NH2   | 50:M4:77:ARG:HA    | 2.31                     | 0.46              |
| 63:N7:105:SER:HA   | 63:N7:108:GLU:HG3  | 1.97                     | 0.46              |
| 64:N8:77:LYS:HB3   | 64:N8:80:THR:OG1   | 2.16                     | 0.46              |
| 78:Q2:61:LYS:HE2   | 78:Q2:63:LYS:O     | 2.16                     | 0.46              |
| 1:6:195:G:H2'      | 1:6:196:G:H5''     | 1.96                     | 0.46              |
| 1:6:570:A:H5''     | 1:6:571:G:OP2      | 2.15                     | 0.46              |
| 1:6:765:G:O6       | 11:s9:149:ARG:HG2  | 2.15                     | 0.46              |
| 1:6:831:U:OP2      | 1:6:831:U:H6       | 1.98                     | 0.46              |
| 3:s1:35:PRO:HB3    | 3:s1:231:LEU:HD11  | 1.98                     | 0.46              |
| 5:s3:72:LEU:HD22   | 12:c0:65:TYR:HD1   | 1.80                     | 0.46              |
| 6:s4:159:THR:HG21  | 6:s4:227:VAL:O     | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:s4:180:LEU:HD13  | 6:s4:228:ILE:HD11  | 1.97                     | 0.46              |
| 10:s8:38:ILE:HA    | 10:s8:60:ILE:O     | 2.15                     | 0.46              |
| 20:c8:15:LEU:HD21  | 20:c8:59:GLY:HA2   | 1.96                     | 0.46              |
| 24:d2:105:THR:HG23 | 24:d2:110:ILE:CG1  | 2.46                     | 0.46              |
| 25:d3:98:GLU:O     | 25:d3:99:ASN:HB2   | 2.15                     | 0.46              |
| 36:5:25:U:O4       | 86:5:3906:OHX:N6   | 2.49                     | 0.46              |
| 36:5:294:U:H4'     | 72:o6:77:LEU:HD23  | 1.97                     | 0.46              |
| 36:5:1560:G:H1     | 36:5:1579:C:H42    | 1.64                     | 0.46              |
| 36:5:1876:U:H5''   | 36:5:1876:U:H6     | 1.80                     | 0.46              |
| 36:5:3310:A:OP1    | 53:m7:74:LYS:NZ    | 2.44                     | 0.46              |
| 41:l4:99:MET:CE    | 41:l4:103:THR:H    | 2.29                     | 0.46              |
| 45:l8:123:GLN:C    | 45:l8:125:ALA:H    | 2.23                     | 0.46              |
| 46:l9:40:HIS:ND1   | 46:l9:41:ILE:HG13  | 2.30                     | 0.46              |
| 47:m0:200:LEU:HD12 | 47:m0:213:PHE:HB2  | 1.96                     | 0.46              |
| 52:m6:65:ASN:HB3   | 52:m6:68:ARG:HD3   | 1.96                     | 0.46              |
| 58:n2:37:LEU:O     | 58:n2:41:ILE:HG13  | 2.15                     | 0.46              |
| 59:n3:54:LEU:HD11  | 59:n3:119:GLY:HA3  | 1.97                     | 0.46              |
| 61:n5:44:PRO:O     | 61:n5:45:LYS:HB2   | 2.16                     | 0.46              |
| 67:o1:19:ARG:HD3   | 67:o1:35:GLU:CG    | 2.45                     | 0.46              |
| 1:2:102:U:O4       | 1:2:360:A:H2'      | 2.16                     | 0.46              |
| 1:2:604:A:OP2      | 86:2:2169:OHX:N5   | 2.48                     | 0.46              |
| 1:2:622:A:OP2      | 86:2:2158:OHX:N1   | 2.49                     | 0.46              |
| 1:2:808:U:H2'      | 1:2:809:A:C8       | 2.51                     | 0.46              |
| 1:2:901:G:C6       | 1:2:902:G:C6       | 3.04                     | 0.46              |
| 1:2:1240:U:OP2     | 86:2:2145:OHX:N1   | 2.49                     | 0.46              |
| 1:2:1615:C:O2'     | 1:2:1616:G:OP2     | 2.32                     | 0.46              |
| 20:C8:126:ARG:HB3  | 20:C8:133:VAL:HG23 | 1.97                     | 0.46              |
| 20:C8:140:THR:HA   | 20:C8:143:ARG:NH1  | 2.31                     | 0.46              |
| 33:E1:126:CYS:O    | 33:E1:128:ALA:N    | 2.47                     | 0.46              |
| 36:1:806:A:H5''    | 36:1:936:A:H61     | 1.81                     | 0.46              |
| 36:1:818:C:N3      | 36:1:920:A:H5'     | 2.31                     | 0.46              |
| 36:1:1683:A:OP2    | 58:N2:85:LYS:HE2   | 2.15                     | 0.46              |
| 36:1:1940:G:H2'    | 36:1:1941:C:O4'    | 2.16                     | 0.46              |
| 36:1:2206:G:H1     | 36:1:2237:C:H42    | 1.63                     | 0.46              |
| 36:1:2947:G:N3     | 40:L3:250:ALA:HB1  | 2.30                     | 0.46              |
| 37:3:24:A:H2'      | 37:3:25:G:O4'      | 2.16                     | 0.46              |
| 37:3:39:C:N3       | 48:M1:70:THR:HG23  | 2.30                     | 0.46              |
| 41:L4:15:ALA:O     | 41:L4:16:THR:OG1   | 2.21                     | 0.46              |
| 41:L4:229:ASN:OD1  | 41:L4:231:ALA:N    | 2.36                     | 0.46              |
| 49:M3:93:ILE:HD13  | 49:M3:93:ILE:HA    | 1.60                     | 0.46              |
| 53:M7:88:VAL:O     | 53:M7:92:GLN:HG2   | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:N7:104:PRO:O   | 63:N7:108:GLU:HG2  | 2.16                     | 0.46              |
| 68:O2:11:LYS:O    | 68:O2:13:HIS:N     | 2.47                     | 0.46              |
| 1:6:263:C:H4'     | 1:6:292:U:H5'      | 1.97                     | 0.46              |
| 1:6:813:U:C6      | 55:m9:163:ARG:HD3  | 2.51                     | 0.46              |
| 1:6:1309:C:O2'    | 1:6:1401:A:N1      | 2.39                     | 0.46              |
| 1:6:1312:A:OP1    | 19:c7:2:GLY:N      | 2.49                     | 0.46              |
| 1:6:1529:C:OP1    | 7:s5:112:ARG:HD3   | 2.16                     | 0.46              |
| 2:s0:179:ARG:HD3  | 2:s0:183:ARG:NE    | 2.30                     | 0.46              |
| 4:s2:246:GLU:H    | 4:s2:246:GLU:HG2   | 1.44                     | 0.46              |
| 13:c1:80:MET:HB3  | 13:c1:83:THR:O     | 2.16                     | 0.46              |
| 14:c2:97:LEU:HD12 | 14:c2:118:ALA:HB3  | 1.96                     | 0.46              |
| 15:c3:74:ILE:O    | 15:c3:78:ASN:ND2   | 2.45                     | 0.46              |
| 21:c9:15:ILE:HD11 | 21:c9:63:ARG:HD3   | 1.97                     | 0.46              |
| 24:d2:74:VAL:O    | 24:d2:75:ILE:HD13  | 2.15                     | 0.46              |
| 34:sR:106:HIS:CD2 | 34:sR:110:VAL:HG22 | 2.50                     | 0.46              |
| 36:5:435:C:H2'    | 36:5:436:A:O4'     | 2.14                     | 0.46              |
| 36:5:985:U:H2'    | 36:5:986:U:H6      | 1.80                     | 0.46              |
| 36:5:2522:G:C6    | 39:l2:70:ARG:NH2   | 2.83                     | 0.46              |
| 40:l3:62:ARG:O    | 40:l3:68:HIS:HB2   | 2.16                     | 0.46              |
| 40:l3:80:ASP:OD2  | 40:l3:314:TYR:OH   | 2.29                     | 0.46              |
| 43:l6:68:PRO:HG2  | 43:l6:71:VAL:HG21  | 1.97                     | 0.46              |
| 44:l7:110:ARG:CZ  | 54:m8:3:ILE:HD12   | 2.45                     | 0.46              |
| 46:l9:122:LYS:HG2 | 46:l9:123:ILE:N    | 2.30                     | 0.46              |
| 68:o2:24:ARG:HG2  | 68:o2:25:TYR:CZ    | 2.50                     | 0.46              |
| 74:o8:14:LEU:C    | 74:o8:16:ARG:H     | 2.23                     | 0.46              |
| 1:2:516:G:OP2     | 86:2:2071:OHX:N6   | 2.48                     | 0.46              |
| 1:2:859:A:C6      | 15:C3:73:ARG:HD3   | 2.49                     | 0.46              |
| 1:2:1194:A:OP2    | 22:D0:75:GLY:N     | 2.48                     | 0.46              |
| 1:2:1427:A:OP2    | 35:SM:93:ARG:NH1   | 2.49                     | 0.46              |
| 24:D2:77:PRO:HG3  | 25:D3:7:ARG:O      | 2.16                     | 0.46              |
| 26:D4:105:ARG:O   | 26:D4:109:LYS:HG3  | 2.16                     | 0.46              |
| 34:SR:13:LEU:HB3  | 34:SR:45:TRP:CZ3   | 2.50                     | 0.46              |
| 36:1:715:A:H4'    | 36:1:716:A:OP1     | 2.15                     | 0.46              |
| 36:1:1555:U:H5''  | 36:1:1556:C:OP2    | 2.16                     | 0.46              |
| 36:1:1796:G:H5''  | 36:1:1797:A:OP1    | 2.16                     | 0.46              |
| 36:1:1947:G:OP1   | 55:M9:136:ARG:NH1  | 2.49                     | 0.46              |
| 36:1:2655:U:C5    | 78:Q2:4:VAL:HG12   | 2.50                     | 0.46              |
| 36:1:2970:C:H4'   | 36:1:2971:A:N1     | 2.31                     | 0.46              |
| 36:1:3154:C:C2    | 36:1:3157:U:O4     | 2.68                     | 0.46              |
| 40:L3:71:GLU:OE1  | 40:L3:357:LYS:NZ   | 2.46                     | 0.46              |
| 40:L3:246:LEU:C   | 40:L3:246:LEU:HD12 | 2.40                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:L4:71:VAL:HG13 | 41:L4:76:ARG:NH1   | 2.30                     | 0.46              |
| 41:L4:148:ILE:HA  | 41:L4:149:PRO:C    | 2.40                     | 0.46              |
| 42:L5:279:LYS:O   | 42:L5:279:LYS:HD3  | 2.16                     | 0.46              |
| 46:L9:25:VAL:HG11 | 46:L9:78:MET:HE1   | 1.97                     | 0.46              |
| 63:N7:17:ARG:HG2  | 70:O4:73:SER:O     | 2.15                     | 0.46              |
| 74:O8:4:GLU:HG2   | 74:O8:5:ILE:H      | 1.80                     | 0.46              |
| 1:6:104:A:H61     | 1:6:308:C:H5'      | 1.81                     | 0.46              |
| 1:6:199:G:HO2'    | 1:6:200:A:H8       | 1.62                     | 0.46              |
| 1:6:968:U:H2'     | 1:6:969:C:O4'      | 2.15                     | 0.46              |
| 1:6:1251:U:H4'    | 33:e1:134:ASN:H    | 1.81                     | 0.46              |
| 1:6:1255:G:H4'    | 1:6:1256:A:OP1     | 2.15                     | 0.46              |
| 3:s1:69:CYS:CB    | 16:c4:114:ARG:HD3  | 2.45                     | 0.46              |
| 6:s4:104:ASP:HB3  | 6:s4:105:VAL:H     | 1.34                     | 0.46              |
| 6:s4:159:THR:HB   | 6:s4:227:VAL:HG23  | 1.97                     | 0.46              |
| 15:c3:151:ASN:O   | 86:c3:201:OHX:N6   | 2.49                     | 0.46              |
| 16:c4:81:VAL:HG13 | 16:c4:115:ILE:HG23 | 1.97                     | 0.46              |
| 22:d0:13:GLU:HG3  | 22:d0:14:GLN:H     | 1.81                     | 0.46              |
| 22:d0:32:LYS:HD2  | 22:d0:32:LYS:H     | 1.80                     | 0.46              |
| 24:d2:7:LEU:HD22  | 24:d2:11:LEU:HG    | 1.97                     | 0.46              |
| 25:d3:60:GLU:CD   | 80:e0:3:LYS:HB2    | 2.41                     | 0.46              |
| 34:sR:111:MET:N   | 34:sR:125:GLY:O    | 2.45                     | 0.46              |
| 36:5:31:C:H4'     | 51:m5:96:ARG:HD3   | 1.98                     | 0.46              |
| 36:5:1235:U:C4'   | 36:5:1236:G:H5'    | 2.45                     | 0.46              |
| 36:5:1349:G:H2'   | 36:5:1350:A:C8     | 2.51                     | 0.46              |
| 36:5:3094:A:H2'   | 36:5:3095:U:C6     | 2.51                     | 0.46              |
| 39:l2:104:LEU:O   | 39:l2:107:VAL:HG22 | 2.16                     | 0.46              |
| 40:l3:168:LYS:O   | 40:l3:319:ASN:ND2  | 2.46                     | 0.46              |
| 44:l7:47:ARG:NH1  | 44:l7:183:ASP:OD2  | 2.49                     | 0.46              |
| 46:l9:87:LYS:HZ3  | 46:l9:191:LEU:HD21 | 1.81                     | 0.46              |
| 51:m5:31:ARG:HG3  | 51:m5:129:TYR:OH   | 2.16                     | 0.46              |
| 53:m7:4:TYR:CE1   | 53:m7:16:SER:HB2   | 2.50                     | 0.46              |
| 1:2:1091:A:N3     | 1:2:1091:A:H5''    | 2.31                     | 0.46              |
| 1:2:1482:C:OP2    | 1:2:1521:G:N1      | 2.45                     | 0.46              |
| 4:S2:178:ILE:HD12 | 4:S2:189:GLN:HG3   | 1.97                     | 0.46              |
| 5:S3:38:GLU:OE1   | 5:S3:40:ARG:NE     | 2.49                     | 0.46              |
| 8:S6:210:GLN:HG2  | 8:S6:214:LYS:HZ2   | 1.80                     | 0.46              |
| 16:C4:29:HIS:HB3  | 16:C4:41:ARG:HG3   | 1.97                     | 0.46              |
| 16:C4:84:ARG:HA   | 16:C4:119:THR:HG22 | 1.97                     | 0.46              |
| 19:C7:71:PHE:HE1  | 19:C7:73:LEU:HD22  | 1.80                     | 0.46              |
| 24:D2:83:ILE:O    | 24:D2:86:ILE:HG12  | 2.16                     | 0.46              |
| 29:D7:50:ALA:O    | 29:D7:52:THR:N     | 2.46                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:1:2261:G:O6     | 86:1:3937:OHX:N4  | 2.48                     | 0.46              |
| 36:1:3084:C:H2'    | 36:1:3085:G:O4'   | 2.15                     | 0.46              |
| 36:1:3214:U:H2'    | 50:M4:121:MET:CE  | 2.46                     | 0.46              |
| 86:1:4056:OHX:N5   | 86:1:4163:OHX:N3  | 2.63                     | 0.46              |
| 41:L4:59:GLN:OE1   | 73:O7:55:ARG:NH2  | 2.45                     | 0.46              |
| 41:L4:144:LYS:O    | 41:L4:144:LYS:HE3 | 2.15                     | 0.46              |
| 42:L5:244:HIS:O    | 42:L5:248:ARG:HG3 | 2.15                     | 0.46              |
| 44:L7:143:THR:HG22 | 44:L7:241:LYS:HE3 | 1.97                     | 0.46              |
| 47:M0:102:MET:HB2  | 47:M0:102:MET:HE3 | 1.57                     | 0.46              |
| 48:M1:32:ARG:O     | 48:M1:36:VAL:HG23 | 2.15                     | 0.46              |
| 59:N3:17:LEU:HD21  | 59:N3:98:ASN:ND2  | 2.31                     | 0.46              |
| 63:N7:50:PRO:HD3   | 63:N7:68:ILE:HG12 | 1.96                     | 0.46              |
| 1:6:470:A:C5'      | 1:6:470:A:H8      | 2.28                     | 0.46              |
| 1:6:486:G:OP1      | 1:6:486:G:H4'     | 2.15                     | 0.46              |
| 1:6:922:G:H4'      | 39:l2:109:GLU:HG3 | 1.98                     | 0.46              |
| 1:6:1053:G:N7      | 86:6:2196:OHX:N4  | 2.63                     | 0.46              |
| 7:s5:29:ILE:HA     | 7:s5:30:PRO:HD3   | 1.82                     | 0.46              |
| 8:s6:63:MET:HE2    | 8:s6:106:LEU:HD22 | 1.98                     | 0.46              |
| 10:s8:154:SER:O    | 10:s8:158:SER:HB3 | 2.16                     | 0.46              |
| 15:c3:85:PRO:HG2   | 15:c3:129:TYR:CE2 | 2.51                     | 0.46              |
| 36:5:2899:C:C5     | 46:l9:171:ASP:HA  | 2.50                     | 0.46              |
| 36:5:3156:U:O2'    | 36:5:3157:U:O2    | 2.33                     | 0.46              |
| 86:5:4033:OHX:N3   | 86:5:4081:OHX:N6  | 2.64                     | 0.46              |
| 86:5:4187:OHX:N1   | 86:5:4189:OHX:N4  | 2.64                     | 0.46              |
| 40:l3:307:PRO:HD3  | 40:l3:311:PHE:CE2 | 2.50                     | 0.46              |
| 42:l5:184:ASP:OD2  | 42:l5:187:THR:OG1 | 2.34                     | 0.46              |
| 64:n8:6:THR:CG2    | 64:n8:8:THR:HG23  | 2.43                     | 0.46              |
| 72:o6:58:ILE:HG22  | 72:o6:90:MET:CG   | 2.44                     | 0.46              |
| 74:o8:17:ARG:HG2   | 74:o8:19:ASP:OD2  | 2.16                     | 0.46              |
| 1:2:142:G:O5'      | 1:2:142:G:C8      | 2.68                     | 0.46              |
| 1:2:386:G:OP2      | 10:S8:25:ARG:NH2  | 2.48                     | 0.46              |
| 1:2:1445:G:N2      | 33:E1:90:LYS:O    | 2.49                     | 0.46              |
| 1:2:1606:C:H2'     | 1:2:1607:G:C8     | 2.51                     | 0.46              |
| 1:2:1649:G:N7      | 86:2:2052:OHX:N1  | 2.64                     | 0.46              |
| 1:2:1662:G:C2'     | 1:2:1663:G:H5'    | 2.46                     | 0.46              |
| 1:2:1748:G:O6      | 86:2:2105:OHX:N4  | 2.49                     | 0.46              |
| 7:S5:117:THR:HG22  | 7:S5:121:ILE:HD11 | 1.98                     | 0.46              |
| 7:S5:143:ARG:NH1   | 7:S5:218:GLU:OE1  | 2.49                     | 0.46              |
| 8:S6:193:LEU:HD23  | 8:S6:193:LEU:HA   | 1.76                     | 0.46              |
| 11:S9:117:GLY:O    | 11:S9:119:ALA:N   | 2.48                     | 0.46              |
| 14:C2:67:THR:C     | 14:C2:69:ALA:H    | 2.24                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:C5:64:LYS:HG3  | 17:C5:73:PRO:HG3   | 1.97                     | 0.46              |
| 33:E1:94:LYS:HB3  | 33:E1:95:HIS:H     | 1.50                     | 0.46              |
| 36:1:291:C:OP1    | 51:M5:68:ARG:NH1   | 2.49                     | 0.46              |
| 36:1:598:A:OP1    | 44:L7:41:ARG:NH1   | 2.48                     | 0.46              |
| 36:1:735:A:H2'    | 36:1:736:A:H8      | 1.78                     | 0.46              |
| 36:1:1221:A:H3'   | 36:1:1222:G:C5'    | 2.45                     | 0.46              |
| 36:1:1454:A:OP2   | 86:1:4210:OHX:N6   | 2.49                     | 0.46              |
| 36:1:2442:G:H2'   | 36:1:2443:A:H5''   | 1.97                     | 0.46              |
| 40:L3:222:LYS:HG2 | 40:L3:223:GLY:N    | 2.30                     | 0.46              |
| 48:M1:150:ASN:C   | 48:M1:152:HIS:H    | 2.23                     | 0.46              |
| 67:O1:19:ARG:HB3  | 67:O1:35:GLU:HG2   | 1.97                     | 0.46              |
| 70:O4:55:SER:HG   | 70:O4:69:HIS:HB3   | 1.80                     | 0.46              |
| 74:O8:32:ASN:HD22 | 74:O8:32:ASN:C     | 2.24                     | 0.46              |
| 1:6:1078:C:H2'    | 1:6:1079:U:C6      | 2.51                     | 0.46              |
| 86:6:2150:OHX:N3  | 86:c1:202:OHX:N5   | 2.63                     | 0.46              |
| 4:s2:186:LYS:HD2  | 4:s2:186:LYS:HA    | 1.86                     | 0.46              |
| 4:s2:188:LEU:HD13 | 4:s2:196:VAL:HG11  | 1.96                     | 0.46              |
| 21:c9:28:LEU:O    | 21:c9:29:GLU:HB2   | 2.15                     | 0.46              |
| 21:c9:118:PRO:C   | 21:c9:120:GLY:H    | 2.23                     | 0.46              |
| 30:d8:26:THR:H    | 30:d8:44:VAL:HG22  | 1.80                     | 0.46              |
| 34:sR:178:VAL:HB  | 34:sR:192:PHE:HB2  | 1.98                     | 0.46              |
| 35:sM:35:ALA:O    | 35:sM:37:VAL:N     | 2.49                     | 0.46              |
| 35:sM:77:THR:C    | 35:sM:79:SER:H     | 2.24                     | 0.46              |
| 36:5:49:A:OP1     | 49:m3:16:LYS:HE3   | 2.16                     | 0.46              |
| 36:5:670:C:OP1    | 54:m8:147:ARG:NH2  | 2.40                     | 0.46              |
| 36:5:1066:G:OP1   | 86:5:4226:OHX:N2   | 2.49                     | 0.46              |
| 36:5:1507:G:N3    | 36:5:1507:G:H5'    | 2.31                     | 0.46              |
| 36:5:2101:C:H2'   | 36:5:2102:U:H6     | 1.81                     | 0.46              |
| 36:5:2581:U:O2'   | 36:5:2582:C:H5'    | 2.15                     | 0.46              |
| 36:5:2747:A:OP1   | 42:l5:176:SER:OG   | 2.33                     | 0.46              |
| 36:5:3216:G:H3'   | 36:5:3219:G:N3     | 2.31                     | 0.46              |
| 86:5:4212:OHX:N2  | 86:5:4222:OHX:N5   | 2.63                     | 0.46              |
| 38:8:145:U:H2'    | 38:8:146:U:H6      | 1.80                     | 0.46              |
| 39:l2:172:GLY:HA3 | 79:q3:67:GLY:HA2   | 1.97                     | 0.46              |
| 40:l3:57:VAL:HG23 | 40:l3:358:TRP:HE3  | 1.81                     | 0.46              |
| 41:l4:104:LYS:HD2 | 41:l4:106:TRP:CZ2  | 2.50                     | 0.46              |
| 45:l8:106:LYS:O   | 45:l8:110:THR:HG23 | 2.16                     | 0.46              |
| 47:m0:24:ARG:O    | 47:m0:25:ALA:HB3   | 2.15                     | 0.46              |
| 51:m5:56:LYS:NZ   | 51:m5:145:ASP:OD2  | 2.40                     | 0.46              |
| 53:m7:25:SER:HB3  | 53:m7:28:ASN:HB2   | 1.97                     | 0.46              |
| 64:n8:7:LYS:HD3   | 64:n8:7:LYS:HA     | 1.72                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:o1:19:ARG:HD3   | 67:o1:35:GLU:HG3   | 1.98                     | 0.46              |
| 68:o2:99:ASN:OD1   | 68:o2:99:ASN:N     | 2.43                     | 0.46              |
| 71:o5:84:LYS:HB3   | 71:o5:85:THR:H     | 1.57                     | 0.46              |
| 77:q1:15:ARG:HG3   | 77:q1:15:ARG:HH11  | 1.81                     | 0.46              |
| 79:q3:56:THR:HB    | 79:q3:63:THR:OG1   | 2.15                     | 0.46              |
| 82:p0:205:THR:C    | 82:p0:207:GLU:H    | 2.24                     | 0.46              |
| 1:2:808:U:O4       | 1:2:809:A:N6       | 2.49                     | 0.46              |
| 1:2:830:U:O2       | 1:2:830:U:H2'      | 2.15                     | 0.46              |
| 1:2:1157:A:C8      | 1:2:1157:A:H3'     | 2.51                     | 0.46              |
| 1:2:1332:C:H6      | 1:2:1332:C:O5'     | 1.99                     | 0.46              |
| 1:2:1490:C:H1'     | 1:2:1491:U:O4'     | 2.15                     | 0.46              |
| 5:S3:64:ARG:O      | 5:S3:66:ILE:N      | 2.49                     | 0.46              |
| 6:S4:192:ILE:HD13  | 6:S4:238:LEU:HD22  | 1.97                     | 0.46              |
| 10:S8:117:TYR:CD1  | 10:S8:150:ALA:HB2  | 2.51                     | 0.46              |
| 19:C7:23:LYS:O     | 19:C7:24:LEU:HB2   | 2.16                     | 0.46              |
| 21:C9:63:ARG:HG3   | 21:C9:67:MET:HE1   | 1.97                     | 0.46              |
| 34:SR:232:TYR:HE1  | 34:SR:234:LEU:HD11 | 1.81                     | 0.46              |
| 36:1:308:A:H5'     | 36:1:2223:A:O2'    | 2.16                     | 0.46              |
| 36:1:908:G:O6      | 36:1:925:A:O2'     | 2.33                     | 0.46              |
| 36:1:1231:A:OP2    | 86:1:4089:OHX:N6   | 2.49                     | 0.46              |
| 36:1:1659:U:H2'    | 36:1:1660:C:C6     | 2.51                     | 0.46              |
| 36:1:1831:U:OP2    | 61:N5:92:LYS:HD2   | 2.16                     | 0.46              |
| 36:1:2158:A:H5'    | 36:1:2160:G:O4'    | 2.15                     | 0.46              |
| 36:1:3192:U:H2'    | 36:1:3193:C:C6     | 2.50                     | 0.46              |
| 39:L2:114:SER:HB2  | 39:L2:169:ILE:CD1  | 2.45                     | 0.46              |
| 40:L3:296:THR:HG21 | 40:L3:357:LYS:C    | 2.41                     | 0.46              |
| 42:L5:56:THR:C     | 42:L5:58:LYS:N     | 2.73                     | 0.46              |
| 45:L8:94:PHE:CE2   | 45:L8:200:LEU:HG   | 2.51                     | 0.46              |
| 46:L9:88:TYR:CE2   | 46:L9:184:LYS:HG2  | 2.51                     | 0.46              |
| 53:M7:41:LEU:HD21  | 53:M7:95:LEU:HD22  | 1.98                     | 0.46              |
| 73:O7:65:ARG:HG3   | 73:O7:65:ARG:HH11  | 1.80                     | 0.46              |
| 1:6:1175:U:H2'     | 1:6:1176:G:C8      | 2.51                     | 0.46              |
| 1:6:1673:G:H8      | 1:6:1673:G:O5'     | 1.98                     | 0.46              |
| 4:s2:243:TYR:HB3   | 4:s2:246:GLU:HG3   | 1.98                     | 0.46              |
| 16:c4:61:MET:HE2   | 16:c4:61:MET:HB3   | 1.81                     | 0.46              |
| 17:c5:72:LYS:H     | 17:c5:72:LYS:HG2   | 1.52                     | 0.46              |
| 18:c6:55:VAL:HG21  | 18:c6:105:LEU:HG   | 1.97                     | 0.46              |
| 20:c8:127:HIS:CD2  | 20:c8:133:VAL:HG11 | 2.51                     | 0.46              |
| 25:d3:12:ALA:O     | 25:d3:16:ARG:HB2   | 2.16                     | 0.46              |
| 35:sM:52:PRO:O     | 35:sM:54:PRO:HD3   | 2.16                     | 0.46              |
| 36:5:209:A:H4'     | 36:5:211:A:C8      | 2.51                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:2655:U:OP2    | 78:q2:2:VAL:HA     | 2.16                     | 0.46              |
| 36:5:2736:A:O2'    | 57:n1:68:THR:HG21  | 2.16                     | 0.46              |
| 36:5:3013:U:H2'    | 36:5:3014:U:C6     | 2.50                     | 0.46              |
| 36:5:3165:A:C6     | 36:5:3286:G:C6     | 3.04                     | 0.46              |
| 37:7:23:A:H2'      | 37:7:24:A:C8       | 2.51                     | 0.46              |
| 37:7:106:U:H2'     | 37:7:107:C:O4'     | 2.16                     | 0.46              |
| 40:l3:10:ARG:NH2   | 40:l3:14:LEU:HD21  | 2.31                     | 0.46              |
| 46:l9:3:TYR:HA     | 56:n0:142:GLN:OE1  | 2.15                     | 0.46              |
| 55:m9:116:ASP:OD1  | 55:m9:116:ASP:N    | 2.40                     | 0.46              |
| 61:n5:105:VAL:HG11 | 61:n5:126:LEU:HD13 | 1.97                     | 0.46              |
| 82:p0:198:PRO:C    | 82:p0:200:SER:H    | 2.24                     | 0.46              |
| 1:2:147:A:H2'      | 1:2:148:A:O4'      | 2.16                     | 0.46              |
| 1:2:647:G:N2       | 1:2:687:G:N2       | 2.64                     | 0.46              |
| 1:2:1266:U:H2'     | 1:2:1267:G:C8      | 2.51                     | 0.46              |
| 86:2:2045:OHX:N2   | 86:2:2099:OHX:N6   | 2.64                     | 0.46              |
| 86:2:2096:OHX:N4   | 86:2:2109:OHX:N2   | 2.64                     | 0.46              |
| 86:2:2172:OHX:N3   | 86:2:2173:OHX:N4   | 2.64                     | 0.46              |
| 3:S1:143:THR:HB    | 3:S1:205:PHE:HE1   | 1.80                     | 0.46              |
| 6:S4:199:GLU:OE2   | 6:S4:209:HIS:NE2   | 2.46                     | 0.46              |
| 9:S7:89:HIS:ND1    | 9:S7:168:SER:OG    | 2.31                     | 0.46              |
| 15:C3:11:ILE:O     | 15:C3:12:SER:HB2   | 2.14                     | 0.46              |
| 17:C5:31:GLU:HG3   | 17:C5:32:ASP:N     | 2.29                     | 0.46              |
| 18:C6:59:LYS:HE2   | 18:C6:59:LYS:HB2   | 1.78                     | 0.46              |
| 20:C8:132:ARG:HG3  | 20:C8:138:THR:HG22 | 1.98                     | 0.46              |
| 22:D0:22:ILE:HG22  | 22:D0:93:LEU:HB2   | 1.96                     | 0.46              |
| 27:D5:39:ALA:HB1   | 27:D5:71:ILE:C     | 2.41                     | 0.46              |
| 27:D5:88:ILE:O     | 27:D5:104:ALA:N    | 2.49                     | 0.46              |
| 34:SR:80:ALA:O     | 34:SR:91:LEU:HD12  | 2.16                     | 0.46              |
| 34:SR:183:LEU:HD23 | 34:SR:183:LEU:HA   | 1.80                     | 0.46              |
| 36:1:307:A:H2'     | 36:1:308:A:C8      | 2.50                     | 0.46              |
| 36:1:1509:A:O2'    | 36:1:1510:G:H5'    | 2.15                     | 0.46              |
| 36:1:1785:U:H2'    | 36:1:1786:G:C8     | 2.51                     | 0.46              |
| 36:1:1856:C:H2'    | 36:1:1857:C:C6     | 2.50                     | 0.46              |
| 36:1:1886:A:O4'    | 36:1:3307:A:H5'    | 2.16                     | 0.46              |
| 36:1:2298:U:O4     | 36:1:2923:U:H5     | 1.99                     | 0.46              |
| 36:1:2533:G:H2'    | 36:1:2534:G:O4'    | 2.15                     | 0.46              |
| 36:1:2617:U:H3'    | 65:N9:3:LYS:HD3    | 1.98                     | 0.46              |
| 86:1:3995:OHX:N1   | 86:1:4034:OHX:N2   | 2.64                     | 0.46              |
| 37:3:40:C:O2'      | 48:M1:72:ARG:HD2   | 2.16                     | 0.46              |
| 40:L3:116:ARG:HG2  | 40:L3:175:LYS:CA   | 2.44                     | 0.46              |
| 41:L4:299:ILE:HG22 | 41:L4:300:ARG:O    | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:L5:215:ASP:OD1  | 42:L5:218:ARG:HG3  | 2.15                     | 0.46              |
| 56:N0:13:ARG:HA    | 56:N0:56:GLY:HA2   | 1.98                     | 0.46              |
| 59:N3:15:LEU:HD23  | 59:N3:53:SER:HB3   | 1.97                     | 0.46              |
| 60:N4:5:ILE:HD12   | 60:N4:10:GLY:HA2   | 1.98                     | 0.46              |
| 68:O2:60:ASN:OD1   | 68:O2:62:LYS:HB2   | 2.15                     | 0.46              |
| 75:O9:23:LEU:HD22  | 75:O9:24:PRO:HD2   | 1.98                     | 0.46              |
| 1:6:492:A:H2'      | 1:6:493:U:H5''     | 1.98                     | 0.46              |
| 7:s5:37:GLN:CD     | 18:c6:53:LEU:HD22  | 2.41                     | 0.46              |
| 22:d0:71:PRO:HB3   | 31:d9:41:GLN:HG2   | 1.98                     | 0.46              |
| 36:5:535:G:P       | 56:n0:146:LYS:HE3  | 2.55                     | 0.46              |
| 86:5:4066:OHX:N1   | 86:5:4141:OHX:N4   | 2.64                     | 0.46              |
| 41:l4:119:ARG:HA   | 41:l4:122:THR:HG23 | 1.97                     | 0.46              |
| 45:l8:108:ARG:HA   | 45:l8:111:LYS:HD2  | 1.98                     | 0.46              |
| 45:l8:169:LEU:HD23 | 45:l8:169:LEU:HA   | 1.81                     | 0.46              |
| 51:m5:27:VAL:HB    | 51:m5:122:ASN:ND2  | 2.31                     | 0.46              |
| 1:2:218:A:HO2'     | 1:2:219:A:P        | 2.32                     | 0.45              |
| 1:2:584:C:OP2      | 86:2:2027:OHX:N6   | 2.49                     | 0.45              |
| 1:2:1754:A:O2'     | 86:2:2059:OHX:N5   | 2.48                     | 0.45              |
| 1:2:1781:A:H2'     | 1:2:1782:A:O4'     | 2.16                     | 0.45              |
| 1:2:1783:C:H2'     | 1:2:1784:C:C6      | 2.50                     | 0.45              |
| 3:S1:71:ALA:HB3    | 16:C4:114:ARG:NH1  | 2.31                     | 0.45              |
| 3:S1:220:GLN:H     | 3:S1:220:GLN:HG3   | 1.47                     | 0.45              |
| 5:S3:30:ALA:C      | 5:S3:32:GLU:H      | 2.24                     | 0.45              |
| 5:S3:211:PRO:HG3   | 19:C7:20:TYR:CE1   | 2.51                     | 0.45              |
| 6:S4:104:ASP:HB2   | 6:S4:108:ARG:H     | 1.81                     | 0.45              |
| 6:S4:121:TYR:HA    | 6:S4:164:LEU:HG    | 1.98                     | 0.45              |
| 6:S4:179:LYS:N     | 6:S4:194:THR:O     | 2.50                     | 0.45              |
| 22:D0:65:ILE:HD11  | 31:D9:36:LEU:HD21  | 1.98                     | 0.45              |
| 34:SR:207:ASP:OD1  | 34:SR:209:THR:OG1  | 2.29                     | 0.45              |
| 36:1:1517:G:P      | 75:O9:41:ARG:HH22  | 2.39                     | 0.45              |
| 36:1:1795:U:H4'    | 36:1:1796:G:C4     | 2.51                     | 0.45              |
| 36:1:2112:U:H5''   | 60:N4:44:LYS:NZ    | 2.30                     | 0.45              |
| 36:1:2513:U:H4'    | 36:1:2514:U:OP1    | 2.16                     | 0.45              |
| 36:1:2558:U:O2'    | 36:1:2559:U:H5'    | 2.16                     | 0.45              |
| 36:1:3079:U:OP1    | 36:1:3079:U:H6     | 1.99                     | 0.45              |
| 86:1:4059:OHX:N2   | 86:1:4166:OHX:N5   | 2.63                     | 0.45              |
| 37:3:27:A:P        | 42:L5:57:ASN:H     | 2.39                     | 0.45              |
| 40:L3:81:THR:HB    | 40:L3:321:PHE:HA   | 1.97                     | 0.45              |
| 45:L8:25:PRO:HG2   | 45:L8:27:THR:HB    | 1.98                     | 0.45              |
| 46:L9:103:ILE:HG12 | 46:L9:136:PHE:CE2  | 2.52                     | 0.45              |
| 46:L9:138:THR:O    | 46:L9:139:ASN:ND2  | 2.39                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:M0:76:MET:CE    | 47:M0:138:VAL:HG11 | 2.46                     | 0.45              |
| 51:M5:31:ARG:NH1   | 51:M5:124:ASP:OD1  | 2.49                     | 0.45              |
| 59:N3:57:MET:HE3   | 59:N3:59:MET:HE1   | 1.98                     | 0.45              |
| 61:N5:38:LEU:CD1   | 61:N5:40:LEU:HD13  | 2.45                     | 0.45              |
| 61:N5:58:ASP:O     | 61:N5:62:VAL:HG23  | 2.16                     | 0.45              |
| 63:N7:17:ARG:C     | 63:N7:19:ALA:H     | 2.24                     | 0.45              |
| 66:O0:30:THR:HB    | 66:O0:91:SER:HB2   | 1.98                     | 0.45              |
| 1:6:234:G:H2'      | 1:6:235:G:O4'      | 2.16                     | 0.45              |
| 1:6:846:G:H2'      | 1:6:847:A:H8       | 1.81                     | 0.45              |
| 1:6:1218:G:O6      | 1:6:1444:A:H2'     | 2.16                     | 0.45              |
| 3:s1:226:GLY:HA2   | 36:5:2536:A:H4'    | 1.98                     | 0.45              |
| 13:c1:46:LYS:HD2   | 13:c1:46:LYS:HA    | 1.61                     | 0.45              |
| 23:d1:60:ARG:HA    | 23:d1:65:SER:HB2   | 1.97                     | 0.45              |
| 31:d9:30:LEU:HA    | 31:d9:39:CYS:HA    | 1.98                     | 0.45              |
| 36:5:577:C:H2'     | 36:5:579:G:H5''    | 1.97                     | 0.45              |
| 36:5:953:G:H2'     | 36:5:1117:G:H5''   | 1.99                     | 0.45              |
| 36:5:1339:C:OP1    | 68:o2:61:LYS:HD3   | 2.16                     | 0.45              |
| 36:5:1363:A:OP2    | 86:5:4197:OHX:N3   | 2.49                     | 0.45              |
| 41:l4:99:MET:HE3   | 41:l4:103:THR:H    | 1.79                     | 0.45              |
| 41:l4:156:LEU:HD23 | 41:l4:159:ILE:HD12 | 1.97                     | 0.45              |
| 43:l6:158:TYR:OH   | 50:m4:114:ASP:OD2  | 2.32                     | 0.45              |
| 57:n1:119:ALA:HB2  | 57:n1:126:VAL:HG13 | 1.98                     | 0.45              |
| 60:n4:82:ILE:O     | 60:n4:82:ILE:HG22  | 2.15                     | 0.45              |
| 62:n6:74:TYR:CE1   | 62:n6:77:LYS:HD2   | 2.50                     | 0.45              |
| 64:n8:66:ALA:HB1   | 64:n8:69:TRP:HB2   | 1.99                     | 0.45              |
| 66:o0:77:LEU:O     | 66:o0:81:VAL:HG22  | 2.16                     | 0.45              |
| 74:o8:22:THR:HG22  | 74:o8:74:LYS:HB3   | 1.98                     | 0.45              |
| 74:o8:30:LYS:HD2   | 74:o8:40:GLN:NE2   | 2.31                     | 0.45              |
| 1:2:61:A:C8        | 1:2:269:G:O2'      | 2.64                     | 0.45              |
| 1:2:649:U:O2'      | 1:2:650:U:H6       | 2.00                     | 0.45              |
| 1:2:987:G:C2       | 39:L2:249:SER:HB2  | 2.52                     | 0.45              |
| 1:2:1316:G:H2'     | 1:2:1317:C:H6      | 1.81                     | 0.45              |
| 1:2:1788:G:P       | 16:C4:127:ARG:HH12 | 2.39                     | 0.45              |
| 86:2:2172:OHX:N5   | 86:2:2173:OHX:N1   | 2.65                     | 0.45              |
| 2:S0:188:LEU:HB3   | 2:S0:189:VAL:H     | 1.57                     | 0.45              |
| 4:S2:42:GLY:HA2    | 4:S2:68:ILE:HD11   | 1.97                     | 0.45              |
| 21:C9:6:VAL:HB     | 21:C9:14:PHE:CE1   | 2.50                     | 0.45              |
| 28:D6:44:ILE:HD12  | 28:D6:45:VAL:HG22  | 1.97                     | 0.45              |
| 33:E1:83:LYS:O     | 33:E1:84:VAL:HG12  | 2.17                     | 0.45              |
| 36:1:107:A:OP1     | 49:M3:39:ARG:NH1   | 2.47                     | 0.45              |
| 36:1:114:A:OP1     | 51:M5:54:LYS:NZ    | 2.49                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:1553:U:H4'   | 36:1:1554:U:H5'    | 1.98                     | 0.45              |
| 36:1:2571:U:OP1   | 36:1:2571:U:H2'    | 2.16                     | 0.45              |
| 36:1:2659:G:N7    | 86:1:3883:OHX:N5   | 2.64                     | 0.45              |
| 86:1:4065:OHX:N4  | 86:1:4177:OHX:N2   | 2.64                     | 0.45              |
| 44:L7:191:VAL:O   | 44:L7:191:VAL:HG12 | 2.16                     | 0.45              |
| 47:M0:170:LYS:NZ  | 47:M0:175:ASN:O    | 2.46                     | 0.45              |
| 48:M1:155:THR:OG1 | 48:M1:158:ASP:HB2  | 2.15                     | 0.45              |
| 55:M9:180:LYS:HA  | 55:M9:183:ALA:HB3  | 1.98                     | 0.45              |
| 61:N5:86:VAL:HG12 | 61:N5:120:LYS:HB3  | 1.99                     | 0.45              |
| 69:O3:49:ILE:HD11 | 69:O3:71:VAL:N     | 2.31                     | 0.45              |
| 73:O7:2:GLY:O     | 73:O7:7:SER:HB3    | 2.16                     | 0.45              |
| 1:6:1769:U:O2     | 16:c4:136:ARG:HD2  | 2.16                     | 0.45              |
| 3:s1:48:VAL:HG22  | 3:s1:64:ARG:NH2    | 2.31                     | 0.45              |
| 3:s1:142:PHE:O    | 3:s1:207:LEU:HA    | 2.17                     | 0.45              |
| 4:s2:245:ASP:N    | 4:s2:245:ASP:OD1   | 2.49                     | 0.45              |
| 8:s6:14:LYS:HG2   | 8:s6:16:PHE:CE2    | 2.51                     | 0.45              |
| 11:s9:109:LEU:HB2 | 11:s9:146:PHE:HB2  | 1.97                     | 0.45              |
| 12:c0:32:HIS:CG   | 12:c0:33:GLU:H     | 2.32                     | 0.45              |
| 18:c6:87:LYS:HE2  | 18:c6:87:LYS:HB3   | 1.76                     | 0.45              |
| 24:d2:28:ARG:HA   | 24:d2:29:PRO:HA    | 1.78                     | 0.45              |
| 27:d5:82:HIS:O    | 27:d5:84:GLU:N     | 2.49                     | 0.45              |
| 36:5:269:G:P      | 51:m5:44:ARG:HH22  | 2.39                     | 0.45              |
| 36:5:566:G:N7     | 86:5:4130:OHX:N5   | 2.65                     | 0.45              |
| 36:5:655:C:H2'    | 36:5:656:A:C8      | 2.51                     | 0.45              |
| 36:5:1481:A:C2'   | 36:5:1858:A:N3     | 2.79                     | 0.45              |
| 36:5:2202:C:H5''  | 39:12:226:SER:N    | 2.32                     | 0.45              |
| 36:5:2403:G:N7    | 36:5:2870:C:H4'    | 2.31                     | 0.45              |
| 36:5:2897:A:H2'   | 36:5:2899:C:H5'    | 1.97                     | 0.45              |
| 86:5:4066:OHX:N5  | 86:5:4141:OHX:N2   | 2.64                     | 0.45              |
| 40:l3:367:LYS:HZ1 | 60:n4:34:SER:H     | 1.64                     | 0.45              |
| 42:l5:90:HIS:NE2  | 42:l5:229:ASP:OD2  | 2.45                     | 0.45              |
| 53:m7:31:GLU:CG   | 53:m7:60:PHE:HA    | 2.46                     | 0.45              |
| 54:m8:62:VAL:O    | 54:m8:87:VAL:HA    | 2.16                     | 0.45              |
| 55:m9:158:GLU:HG2 | 55:m9:158:GLU:H    | 1.58                     | 0.45              |
| 59:n3:11:PHE:CD1  | 59:n3:88:ARG:HD2   | 2.51                     | 0.45              |
| 70:o4:81:CYS:SG   | 70:o4:84:CYS:SG    | 3.06                     | 0.45              |
| 1:2:1347:U:O2     | 1:2:1516:A:H5'     | 2.17                     | 0.45              |
| 1:2:1738:U:H2'    | 1:2:1739:C:C6      | 2.51                     | 0.45              |
| 86:2:2084:OHX:N6  | 86:2:2086:OHX:N5   | 2.65                     | 0.45              |
| 6:S4:222:LEU:O    | 6:S4:225:VAL:N     | 2.47                     | 0.45              |
| 6:S4:246:LEU:HD21 | 6:S4:254:ARG:CZ    | 2.46                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:S5:76:ARG:NH2    | 18:C6:120:ASP:OD1  | 2.49                     | 0.45              |
| 21:C9:63:ARG:O     | 21:C9:67:MET:HE3   | 2.16                     | 0.45              |
| 21:C9:108:LEU:HA   | 21:C9:111:ILE:HG22 | 1.98                     | 0.45              |
| 22:D0:105:GLN:HG3  | 22:D0:106:ILE:H    | 1.80                     | 0.45              |
| 22:D0:108:ILE:H    | 22:D0:108:ILE:HG13 | 1.60                     | 0.45              |
| 30:D8:66:LEU:HD23  | 30:D8:66:LEU:HA    | 1.73                     | 0.45              |
| 36:1:29:C:H4'      | 36:1:62:A:H4'      | 1.98                     | 0.45              |
| 36:1:410:U:O4      | 86:1:4060:OHX:N2   | 2.50                     | 0.45              |
| 36:1:1362:G:H2'    | 36:1:1363:A:C8     | 2.52                     | 0.45              |
| 36:1:1915:A:H2'    | 36:1:1916:U:C6     | 2.51                     | 0.45              |
| 36:1:2383:C:H5'    | 52:M6:71:PHE:CE2   | 2.52                     | 0.45              |
| 36:1:2407:C:H2'    | 36:1:2408:U:H6     | 1.81                     | 0.45              |
| 36:1:2767:U:P      | 86:1:4136:OHX:N2   | 2.89                     | 0.45              |
| 36:1:2877:G:H2'    | 36:1:2878:G:O4'    | 2.16                     | 0.45              |
| 36:1:3065:G:O6     | 86:1:4138:OHX:N6   | 2.48                     | 0.45              |
| 36:1:3088:G:H2'    | 36:1:3089:C:O4'    | 2.16                     | 0.45              |
| 36:1:3121:U:H1'    | 36:1:3122:A:H5''   | 1.97                     | 0.45              |
| 36:1:3139:A:H2'    | 36:1:3140:G:O4'    | 2.17                     | 0.45              |
| 36:1:3257:C:H2'    | 36:1:3258:U:O4'    | 2.16                     | 0.45              |
| 40:L3:102:LEU:HD23 | 40:L3:102:LEU:N    | 2.28                     | 0.45              |
| 41:L4:16:THR:HG22  | 41:L4:18:ASN:HB3   | 1.99                     | 0.45              |
| 42:L5:95:TRP:CH2   | 42:L5:161:GLY:HA2  | 2.51                     | 0.45              |
| 44:L7:244:ASN:C    | 44:L7:244:ASN:ND2  | 2.72                     | 0.45              |
| 55:M9:13:SER:OG    | 55:M9:38:ARG:NH2   | 2.49                     | 0.45              |
| 55:M9:15:VAL:HG11  | 55:M9:52:LYS:HG3   | 1.97                     | 0.45              |
| 60:N4:17:ARG:HA    | 60:N4:17:ARG:HD3   | 1.73                     | 0.45              |
| 63:N7:54:THR:OG1   | 63:N7:55:LYS:N     | 2.50                     | 0.45              |
| 78:Q2:40:LYS:HE3   | 78:Q2:44:ASP:OD2   | 2.17                     | 0.45              |
| 1:6:57:G:OP1       | 26:d4:112:LYS:NZ   | 2.48                     | 0.45              |
| 1:6:121:U:H1'      | 6:s4:33:ALA:O      | 2.17                     | 0.45              |
| 1:6:180:A:H2'      | 1:6:181:A:O4'      | 2.16                     | 0.45              |
| 1:6:794:U:H3'      | 1:6:795:U:H5'      | 1.98                     | 0.45              |
| 1:6:1154:G:N7      | 86:6:2135:OHX:N2   | 2.65                     | 0.45              |
| 4:s2:187:LEU:HD12  | 4:s2:211:LEU:HD22  | 1.98                     | 0.45              |
| 13:c1:101:GLU:OE1  | 25:d3:16:ARG:NH2   | 2.50                     | 0.45              |
| 15:c3:80:LEU:HD12  | 15:c3:80:LEU:HA    | 1.76                     | 0.45              |
| 16:c4:119:THR:HA   | 16:c4:120:PRO:HD2  | 1.64                     | 0.45              |
| 18:c6:129:PHE:CE1  | 22:d0:78:THR:HA    | 2.51                     | 0.45              |
| 36:5:298:U:H5''    | 36:5:299:G:H5'     | 1.97                     | 0.45              |
| 36:5:361:A:OP1     | 73:o7:24:ARG:NH1   | 2.49                     | 0.45              |
| 36:5:595:G:H1      | 36:5:609:G:H5''    | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:708:G:H5''    | 36:5:708:G:H8      | 1.81                     | 0.45              |
| 36:5:1064:A:H4'    | 36:5:1065:A:O5'    | 2.16                     | 0.45              |
| 36:5:2093:A:O2'    | 36:5:2094:C:O4'    | 2.24                     | 0.45              |
| 36:5:2440:G:H2'    | 36:5:2441:A:C8     | 2.51                     | 0.45              |
| 36:5:2585:G:C2     | 38:8:151:C:H5      | 2.35                     | 0.45              |
| 36:5:2700:G:O2'    | 36:5:2705:A:N1     | 2.47                     | 0.45              |
| 36:5:2883:U:OP2    | 86:5:4061:OHX:N4   | 2.50                     | 0.45              |
| 37:7:13:A:N3       | 42:15:24:ARG:NH2   | 2.64                     | 0.45              |
| 38:8:1:A:OP1       | 86:8:214:OHX:N5    | 2.50                     | 0.45              |
| 39:12:147:ARG:NH2  | 39:12:155:LYS:HG3  | 2.25                     | 0.45              |
| 40:13:35:ASP:OD2   | 40:13:37:ARG:HD2   | 2.16                     | 0.45              |
| 40:13:147:GLU:OE1  | 40:13:150:ARG:NH2  | 2.49                     | 0.45              |
| 40:13:169:THR:HG23 | 40:13:171:LEU:H    | 1.80                     | 0.45              |
| 43:16:100:LYS:NZ   | 43:16:133:GLU:OE1  | 2.47                     | 0.45              |
| 44:17:47:ARG:NH2   | 44:17:179:LEU:HD11 | 2.32                     | 0.45              |
| 51:m5:44:ARG:HB2   | 51:m5:47:LYS:HB3   | 1.99                     | 0.45              |
| 54:m8:120:GLU:OE2  | 54:m8:130:ARG:NH2  | 2.25                     | 0.45              |
| 59:n3:40:LYS:O     | 59:n3:41:GLY:C     | 2.57                     | 0.45              |
| 64:n8:62:HIS:CG    | 64:n8:62:HIS:O     | 2.68                     | 0.45              |
| 68:o2:19:ARG:HD2   | 68:o2:28:VAL:CG1   | 2.47                     | 0.45              |
| 2:S0:111:ILE:HD12  | 2:S0:111:ILE:HA    | 1.71                     | 0.45              |
| 7:S5:42:LEU:HB2    | 7:S5:46:TRP:O      | 2.16                     | 0.45              |
| 10:S8:26:LYS:O     | 10:S8:29:LEU:HB3   | 2.17                     | 0.45              |
| 14:C2:74:LEU:HD11  | 33:E1:106:TYR:CD1  | 2.50                     | 0.45              |
| 21:C9:40:SER:OG    | 21:C9:96:ALA:HA    | 2.16                     | 0.45              |
| 21:C9:77:ASN:OD1   | 21:C9:101:ASN:ND2  | 2.49                     | 0.45              |
| 23:D1:36:VAL:HG11  | 23:D1:78:LEU:HD13  | 1.98                     | 0.45              |
| 25:D3:7:ARG:HG2    | 25:D3:7:ARG:HH11   | 1.81                     | 0.45              |
| 26:D4:60:PHE:CD1   | 26:D4:71:GLY:HA3   | 2.51                     | 0.45              |
| 32:E0:56:MET:C     | 32:E0:58:PRO:HD3   | 2.40                     | 0.45              |
| 36:1:330:G:OP2     | 86:1:4046:OHX:N2   | 2.49                     | 0.45              |
| 36:1:505:G:OP1     | 41:L4:320:ASN:ND2  | 2.39                     | 0.45              |
| 36:1:627:U:H4'     | 36:1:1399:A:O2'    | 2.17                     | 0.45              |
| 36:1:847:A:H2'     | 36:1:848:A:C8      | 2.51                     | 0.45              |
| 36:1:1495:U:H5     | 36:1:1835:A:C2     | 2.35                     | 0.45              |
| 36:1:2225:U:H2'    | 36:1:2226:U:H6     | 1.79                     | 0.45              |
| 36:1:2746:A:C6     | 42:L5:148:ILE:HD12 | 2.50                     | 0.45              |
| 39:L2:230:VAL:O    | 39:L2:233:GLN:HB2  | 2.16                     | 0.45              |
| 40:L3:71:GLU:OE1   | 60:N4:1:MET:N      | 2.47                     | 0.45              |
| 40:L3:106:TRP:HB2  | 40:L3:133:TYR:CE2  | 2.51                     | 0.45              |
| 40:L3:243:HIS:C    | 40:L3:244:ARG:HG3  | 2.42                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:L3:283:TYR:HB2 | 40:L3:323:MET:HE2  | 1.98                     | 0.45              |
| 43:L6:3:ALA:HB2   | 68:O2:77:ALA:HB2   | 1.98                     | 0.45              |
| 48:M1:23:VAL:HG13 | 48:M1:29:ARG:HH11  | 1.81                     | 0.45              |
| 50:M4:8:LYS:HB3   | 50:M4:9:ALA:H      | 1.55                     | 0.45              |
| 51:M5:180:PHE:O   | 51:M5:184:LYS:HB2  | 2.16                     | 0.45              |
| 53:M7:36:ILE:HG12 | 53:M7:44:ALA:HB1   | 1.98                     | 0.45              |
| 57:N1:75:ILE:HG22 | 57:N1:88:ARG:HD2   | 1.98                     | 0.45              |
| 59:N3:62:VAL:HG23 | 59:N3:74:MET:HE1   | 1.99                     | 0.45              |
| 59:N3:74:MET:SD   | 59:N3:102:ILE:HD13 | 2.57                     | 0.45              |
| 59:N3:120:LYS:H   | 59:N3:137:VAL:CG2  | 2.30                     | 0.45              |
| 60:N4:23:ARG:NH2  | 60:N4:25:ASP:OD2   | 2.48                     | 0.45              |
| 64:N8:84:GLU:HA   | 64:N8:87:ARG:HB2   | 1.98                     | 0.45              |
| 1:6:658:C:H5'     | 1:6:659:C:OP2      | 2.16                     | 0.45              |
| 2:s0:160:ILE:HA   | 2:s0:161:PRO:HD2   | 1.85                     | 0.45              |
| 3:s1:51:SER:HB3   | 3:s1:57:ALA:H      | 1.81                     | 0.45              |
| 6:s4:62:LYS:HE3   | 6:s4:66:MET:CG     | 2.47                     | 0.45              |
| 9:s7:46:ILE:HG12  | 9:s7:60:ILE:HA     | 1.99                     | 0.45              |
| 9:s7:74:GLN:HG2   | 9:s7:131:PHE:CD2   | 2.51                     | 0.45              |
| 9:s7:96:ARG:CZ    | 9:s7:124:LYS:HB3   | 2.47                     | 0.45              |
| 16:c4:99:GLN:HG3  | 28:d6:46:GLU:OE2   | 2.16                     | 0.45              |
| 19:c7:34:LEU:HD22 | 19:c7:38:ILE:HD13  | 1.97                     | 0.45              |
| 20:c8:11:PHE:CD1  | 27:d5:41:ILE:HD13  | 2.51                     | 0.45              |
| 21:c9:105:LEU:O   | 21:c9:109:GLU:HG3  | 2.16                     | 0.45              |
| 22:d0:51:VAL:O    | 22:d0:52:LYS:HB2   | 2.17                     | 0.45              |
| 25:d3:132:LEU:O   | 25:d3:136:TRP:N    | 2.40                     | 0.45              |
| 34:sR:112:SER:HB2 | 34:sR:153:GLN:HA   | 1.98                     | 0.45              |
| 34:sR:200:ASN:N   | 34:sR:214:ALA:O    | 2.49                     | 0.45              |
| 36:5:1368:U:H5'   | 68:o2:43:ARG:NH1   | 2.31                     | 0.45              |
| 36:5:2217:U:H2'   | 36:5:2218:G:H8     | 1.81                     | 0.45              |
| 36:5:2505:U:H2'   | 36:5:2506:U:C5     | 2.51                     | 0.45              |
| 36:5:3154:C:O2    | 36:5:3154:C:H2'    | 2.17                     | 0.45              |
| 41:l4:141:ARG:CZ  | 41:l4:180:LYS:HD3  | 2.47                     | 0.45              |
| 44:l7:221:LYS:O   | 44:l7:228:SER:O    | 2.35                     | 0.45              |
| 45:l8:113:ALA:C   | 45:l8:115:ALA:H    | 2.22                     | 0.45              |
| 59:n3:45:ARG:O    | 59:n3:46:LEU:C     | 2.59                     | 0.45              |
| 68:o2:40:SER:O    | 68:o2:44:ARG:HG3   | 2.16                     | 0.45              |
| 76:q0:88:LYS:HE3  | 76:q0:88:LYS:HB3   | 1.46                     | 0.45              |
| 1:2:420:A:H2'     | 1:2:421:A:O4'      | 2.17                     | 0.45              |
| 1:2:943:C:N4      | 28:D6:15:ARG:HG2   | 2.31                     | 0.45              |
| 1:2:1057:U:H1'    | 1:2:1058:U:H2'     | 1.99                     | 0.45              |
| 3:S1:105:PHE:CD2  | 3:S1:213:ARG:HA    | 2.52                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:S1:190:PRO:C    | 3:S1:191:GLU:HG2   | 2.42                     | 0.45              |
| 4:S2:178:ILE:HB   | 4:S2:185:LYS:HE3   | 1.98                     | 0.45              |
| 8:S6:21:GLU:O     | 8:S6:25:ARG:HB2    | 2.17                     | 0.45              |
| 11:S9:119:ALA:HA  | 11:S9:124:HIS:HD2  | 1.80                     | 0.45              |
| 13:C1:6:THR:HB    | 13:C1:9:SER:HB3    | 1.98                     | 0.45              |
| 14:C2:24:ILE:O    | 14:C2:26:ASP:N     | 2.50                     | 0.45              |
| 16:C4:87:GLY:O    | 16:C4:90:ARG:HB2   | 2.16                     | 0.45              |
| 21:C9:118:PRO:C   | 21:C9:120:GLY:H    | 2.24                     | 0.45              |
| 29:D7:37:CYS:O    | 29:D7:39:GLY:N     | 2.50                     | 0.45              |
| 33:E1:117:LEU:HB3 | 33:E1:118:ARG:NH1  | 2.30                     | 0.45              |
| 34:SR:33:LEU:O    | 34:SR:45:TRP:HD1   | 1.99                     | 0.45              |
| 36:1:2516:U:O2'   | 36:1:2595:A:N6     | 2.47                     | 0.45              |
| 41:L4:157:GLU:HB3 | 41:L4:211:GLU:O    | 2.17                     | 0.45              |
| 41:L4:269:SER:O   | 41:L4:269:SER:OG   | 2.19                     | 0.45              |
| 42:L5:55:PHE:CZ   | 42:L5:158:ARG:HG3  | 2.52                     | 0.45              |
| 43:L6:58:LEU:HD12 | 43:L6:78:ARG:HD3   | 1.98                     | 0.45              |
| 44:L7:152:GLY:O   | 44:L7:163:LEU:HG   | 2.17                     | 0.45              |
| 52:M6:31:GLN:HG3  | 52:M6:33:ILE:HD12  | 1.99                     | 0.45              |
| 58:N2:100:THR:O   | 58:N2:101:ASN:HB2  | 2.17                     | 0.45              |
| 61:N5:76:VAL:HG22 | 61:N5:81:ILE:O     | 2.16                     | 0.45              |
| 67:O1:23:VAL:O    | 67:O1:28:ARG:NH1   | 2.47                     | 0.45              |
| 1:6:56:U:H4'      | 1:6:57:G:H5'       | 1.97                     | 0.45              |
| 2:s0:172:LEU:HD22 | 2:s0:176:LEU:HG    | 1.99                     | 0.45              |
| 5:s3:21:LEU:HD22  | 5:s3:25:PHE:CE2    | 2.52                     | 0.45              |
| 5:s3:195:SER:HB2  | 5:s3:200:LYS:HG2   | 1.99                     | 0.45              |
| 5:s3:210:GLU:HA   | 5:s3:211:PRO:HD3   | 1.83                     | 0.45              |
| 6:s4:125:LYS:HB2  | 6:s4:226:PHE:CE2   | 2.52                     | 0.45              |
| 7:s5:41:LYS:HB3   | 7:s5:41:LYS:HE2    | 1.55                     | 0.45              |
| 31:d9:21:CYS:HA   | 31:d9:30:LEU:HD21  | 1.98                     | 0.45              |
| 36:5:746:A:OP1    | 54:m8:145:ASN:ND2  | 2.50                     | 0.45              |
| 36:5:1560:G:C6    | 36:5:1580:A:N6     | 2.85                     | 0.45              |
| 36:5:1564:U:H2'   | 36:5:1565:G:C8     | 2.52                     | 0.45              |
| 36:5:2101:C:H2'   | 36:5:2102:U:C6     | 2.51                     | 0.45              |
| 36:5:2724:U:H4'   | 57:n1:54:HIS:CD2   | 2.51                     | 0.45              |
| 36:5:2960:C:OP1   | 86:5:3972:OHX:N5   | 2.50                     | 0.45              |
| 86:5:4201:OHX:N2  | 86:8:224:OHX:N5    | 2.64                     | 0.45              |
| 37:7:2:G:H5'      | 42:l5:270:LYS:HG2  | 1.98                     | 0.45              |
| 40:l3:84:VAL:HG13 | 40:l3:162:VAL:HB   | 1.97                     | 0.45              |
| 42:l5:119:TYR:CZ  | 42:l5:135:VAL:HG23 | 2.52                     | 0.45              |
| 42:l5:269:SER:O   | 42:l5:270:LYS:HB2  | 2.16                     | 0.45              |
| 43:l6:42:LEU:HD23 | 43:l6:84:VAL:HG22  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:l9:84:LYS:HA    | 46:l9:188:THR:HB  | 1.99                     | 0.45              |
| 74:o8:17:ARG:NH2   | 74:o8:52:TYR:OH   | 2.45                     | 0.45              |
| 1:2:830:U:O2'      | 1:2:831:U:OP2     | 2.31                     | 0.45              |
| 1:2:1469:A:H2'     | 1:2:1470:C:C6     | 2.52                     | 0.45              |
| 3:S1:77:GLU:C      | 3:S1:79:HIS:N     | 2.74                     | 0.45              |
| 3:S1:116:LYS:HB3   | 3:S1:117:TRP:H    | 1.65                     | 0.45              |
| 6:S4:86:PHE:O      | 6:S4:87:MET:HB2   | 2.16                     | 0.45              |
| 7:S5:25:LEU:HD22   | 7:S5:25:LEU:H     | 1.81                     | 0.45              |
| 10:S8:184:LEU:HD12 | 10:S8:184:LEU:HA  | 1.83                     | 0.45              |
| 16:C4:117:ASP:OD1  | 16:C4:118:VAL:N   | 2.49                     | 0.45              |
| 16:C4:126:THR:O    | 16:C4:127:ARG:C   | 2.59                     | 0.45              |
| 17:C5:123:TYR:HD2  | 17:C5:124:THR:O   | 1.98                     | 0.45              |
| 23:D1:80:LYS:O     | 23:D1:81:ASN:HB2  | 2.17                     | 0.45              |
| 35:SM:47:ALA:HB2   | 36:1:2678:A:C8    | 2.51                     | 0.45              |
| 36:1:551:A:C4      | 36:1:552:G:C8     | 3.05                     | 0.45              |
| 36:1:655:C:H2'     | 36:1:656:A:H8     | 1.80                     | 0.45              |
| 36:1:1554:U:O2'    | 36:1:1582:C:H5    | 1.98                     | 0.45              |
| 36:1:3039:C:OP1    | 59:N3:88:ARG:NH2  | 2.50                     | 0.45              |
| 40:L3:40:PRO:C     | 40:L3:185:GLY:HA3 | 2.42                     | 0.45              |
| 40:L3:107:ALA:HA   | 40:L3:199:PHE:CD2 | 2.50                     | 0.45              |
| 40:L3:214:MET:HE2  | 40:L3:350:ALA:HB2 | 1.98                     | 0.45              |
| 42:L5:150:LEU:HD23 | 42:L5:150:LEU:HA  | 1.75                     | 0.45              |
| 44:L7:177:GLY:O    | 44:L7:178:ILE:HB  | 2.16                     | 0.45              |
| 45:L8:41:GLN:HG3   | 45:L8:44:ARG:NH1  | 2.31                     | 0.45              |
| 57:N1:83:ARG:HD2   | 57:N1:85:LEU:HD21 | 1.98                     | 0.45              |
| 78:Q2:50:PHE:O     | 86:Q2:503:OHX:N2  | 2.49                     | 0.45              |
| 1:6:219:A:C6       | 1:6:843:U:H1'     | 2.52                     | 0.45              |
| 1:6:272:U:O2'      | 1:6:273:G:OP2     | 2.28                     | 0.45              |
| 1:6:1332:C:H4'     | 5:s3:203:PRO:HB3  | 1.99                     | 0.45              |
| 86:6:2067:OHX:N3   | 86:6:2075:OHX:N5  | 2.65                     | 0.45              |
| 4:s2:54:GLU:OE1    | 23:d1:11:LEU:HB2  | 2.16                     | 0.45              |
| 5:s3:34:TYR:HE2    | 5:s3:37:VAL:HG13  | 1.81                     | 0.45              |
| 7:s5:122:ASN:ND2   | 7:s5:126:ASP:O    | 2.45                     | 0.45              |
| 8:s6:164:LYS:HB3   | 8:s6:167:LYS:O    | 2.17                     | 0.45              |
| 8:s6:214:LYS:C     | 8:s6:216:LEU:H    | 2.23                     | 0.45              |
| 16:c4:88:GLY:O     | 16:c4:92:LYS:NZ   | 2.49                     | 0.45              |
| 17:c5:18:ARG:NH2   | 17:c5:38:PRO:HG3  | 2.31                     | 0.45              |
| 19:c7:5:ARG:O      | 19:c7:10:LYS:HE2  | 2.17                     | 0.45              |
| 24:d2:24:GLN:NE2   | 29:d7:3:LEU:O     | 2.40                     | 0.45              |
| 34:sR:194:GLY:HA3  | 34:sR:221:MET:HE1 | 1.99                     | 0.45              |
| 36:5:10:C:O2'      | 36:5:1558:A:N6    | 2.46                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:l3:56:ILE:HG12  | 40:l3:356:LEU:HD22 | 1.97                     | 0.45              |
| 43:l6:2:SER:HA     | 68:o2:81:ASP:OD2   | 2.16                     | 0.45              |
| 54:m8:100:THR:HG23 | 54:m8:120:GLU:HB3  | 1.97                     | 0.45              |
| 57:n1:56:PHE:CE1   | 57:n1:78:LYS:HD3   | 2.51                     | 0.45              |
| 59:n3:13:ILE:HG13  | 59:n3:14:SER:N     | 2.23                     | 0.45              |
| 61:n5:115:ARG:HG3  | 61:n5:115:ARG:NH1  | 2.32                     | 0.45              |
| 66:o0:10:ILE:HD13  | 66:o0:104:LEU:HD21 | 1.98                     | 0.45              |
| 66:o0:18:ILE:HG13  | 66:o0:23:TYR:CE1   | 2.52                     | 0.45              |
| 71:o5:73:LYS:HA    | 71:o5:73:LYS:HD2   | 1.63                     | 0.45              |
| 82:p0:37:GLN:NE2   | 82:p0:184:GLY:HA2  | 2.31                     | 0.45              |
| 1:2:144:U:O2'      | 1:2:145:A:H8       | 1.99                     | 0.45              |
| 1:2:383:G:N7       | 86:2:2131:OHX:N4   | 2.64                     | 0.45              |
| 1:2:477:A:H61      | 1:2:511:A:H61      | 1.64                     | 0.45              |
| 1:2:830:U:O2'      | 1:2:831:U:H6       | 1.98                     | 0.45              |
| 1:2:1433:G:C8      | 31:D9:41:GLN:HG2   | 2.51                     | 0.45              |
| 2:S0:58:VAL:O      | 2:S0:62:ARG:HB2    | 2.16                     | 0.45              |
| 3:S1:88:VAL:HG11   | 3:S1:96:LEU:HD12   | 1.96                     | 0.45              |
| 3:S1:126:THR:HG22  | 3:S1:136:ARG:HB2   | 1.99                     | 0.45              |
| 4:S2:35:TRP:CD1    | 4:S2:35:TRP:C      | 2.94                     | 0.45              |
| 7:S5:59:VAL:O      | 7:S5:60:ASP:HB2    | 2.17                     | 0.45              |
| 12:C0:7:ASP:O      | 12:C0:11:ILE:HG12  | 2.16                     | 0.45              |
| 19:C7:106:THR:O    | 19:C7:110:VAL:HG23 | 2.17                     | 0.45              |
| 22:D0:48:HIS:O     | 22:D0:48:HIS:CG    | 2.70                     | 0.45              |
| 36:1:385:A:H2'     | 36:1:386:A:H8      | 1.80                     | 0.45              |
| 36:1:1879:A:H4'    | 36:1:1880:U:OP2    | 2.15                     | 0.45              |
| 36:1:2943:G:P      | 40:L3:2:SER:HB2    | 2.56                     | 0.45              |
| 86:1:4065:OHX:N6   | 86:1:4177:OHX:N5   | 2.65                     | 0.45              |
| 86:1:4088:OHX:N6   | 86:1:4157:OHX:N4   | 2.64                     | 0.45              |
| 40:L3:41:VAL:CA    | 40:L3:185:GLY:HA3  | 2.46                     | 0.45              |
| 42:L5:119:TYR:CE1  | 42:L5:135:VAL:HG23 | 2.52                     | 0.45              |
| 46:L9:105:GLU:OE2  | 46:L9:108:GLY:HA2  | 2.17                     | 0.45              |
| 61:N5:106:ASP:O    | 61:N5:127:THR:HG23 | 2.16                     | 0.45              |
| 72:O6:26:ILE:H     | 72:O6:26:ILE:HG13  | 1.51                     | 0.45              |
| 1:6:53:G:H2'       | 1:6:54:C:O4'       | 2.16                     | 0.45              |
| 1:6:73:U:H2'       | 1:6:74:U:C6        | 2.50                     | 0.45              |
| 1:6:591:A:H2'      | 1:6:592:A:C8       | 2.51                     | 0.45              |
| 1:6:716:C:H2'      | 1:6:717:C:O4'      | 2.17                     | 0.45              |
| 1:6:967:A:OP2      | 15:c3:124:ARG:NH2  | 2.43                     | 0.45              |
| 1:6:994:G:O2'      | 1:6:995:A:H5'      | 2.17                     | 0.45              |
| 1:6:1122:G:O6      | 86:6:2162:OHX:N6   | 2.50                     | 0.45              |
| 2:s0:179:ARG:O     | 2:s0:183:ARG:HD3   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:s3:10:LYS:HG3    | 5:s3:11:LEU:HD23   | 1.98                     | 0.45              |
| 7:s5:45:LYS:HD3    | 7:s5:45:LYS:HA     | 1.41                     | 0.45              |
| 14:c2:45:LEU:O     | 14:c2:49:THR:HG23  | 2.16                     | 0.45              |
| 18:c6:54:LEU:HD21  | 18:c6:112:TYR:CE1  | 2.52                     | 0.45              |
| 24:d2:119:LYS:HB2  | 24:d2:121:VAL:HG22 | 1.99                     | 0.45              |
| 34:sR:76:ASP:OD1   | 34:sR:76:ASP:N     | 2.47                     | 0.45              |
| 35:sM:23:LYS:HA    | 35:sM:23:LYS:HD2   | 1.71                     | 0.45              |
| 36:5:1781:C:H2'    | 36:5:1782:U:H6     | 1.79                     | 0.45              |
| 36:5:2137:U:C6     | 36:5:2141:U:C4     | 3.05                     | 0.45              |
| 36:5:2439:A:N6     | 36:5:2508:U:H3     | 2.14                     | 0.45              |
| 36:5:2606:G:H2'    | 36:5:2606:G:N3     | 2.31                     | 0.45              |
| 36:5:3364:C:OP1    | 86:5:3942:OHX:N1   | 2.50                     | 0.45              |
| 37:7:22:A:N1       | 42:l5:269:SER:O    | 2.50                     | 0.45              |
| 42:l5:95:TRP:HZ3   | 42:l5:156:GLY:O    | 2.00                     | 0.45              |
| 45:l8:140:VAL:O    | 45:l8:144:GLU:HG3  | 2.16                     | 0.45              |
| 47:m0:175:ASN:O    | 47:m0:176:LEU:HB2  | 2.16                     | 0.45              |
| 47:m0:218:ALA:O    | 86:m0:301:OHX:N3   | 2.49                     | 0.45              |
| 49:m3:46:ILE:HG22  | 49:m3:49:ARG:CB    | 2.34                     | 0.45              |
| 50:m4:31:LYS:HD3   | 50:m4:51:ALA:HB1   | 1.98                     | 0.45              |
| 51:m5:73:ARG:O     | 51:m5:75:VAL:N     | 2.48                     | 0.45              |
| 82:p0:97:LYS:HG3   | 82:p0:98:ASN:N     | 2.32                     | 0.45              |
| 1:2:380:U:H5       | 11:S9:5:PRO:CA     | 2.29                     | 0.45              |
| 1:2:1300:A:P       | 4:S2:99:LYS:HZ1    | 2.39                     | 0.45              |
| 1:2:1509:C:H2'     | 1:2:1510:U:O4'     | 2.16                     | 0.45              |
| 86:2:2116:OHX:N2   | 86:C1:201:OHX:N4   | 2.64                     | 0.45              |
| 4:S2:97:ARG:HB2    | 4:S2:118:ALA:O     | 2.17                     | 0.45              |
| 5:S3:164:VAL:O     | 5:S3:168:ILE:HG13  | 2.16                     | 0.45              |
| 15:C3:91:LEU:HB3   | 15:C3:122:ILE:HG12 | 1.98                     | 0.45              |
| 18:C6:143:ARG:HH22 | 35:SM:84:LYS:NZ    | 2.14                     | 0.45              |
| 25:D3:142:LYS:HA   | 25:D3:143:PRO:HD3  | 1.82                     | 0.45              |
| 31:D9:7:TRP:O      | 31:D9:8:PHE:HB2    | 2.15                     | 0.45              |
| 34:SR:154:VAL:HG12 | 34:SR:171:SER:CB   | 2.46                     | 0.45              |
| 36:1:1094:U:O2'    | 36:1:1095:U:O5'    | 2.31                     | 0.45              |
| 36:1:1230:G:N2     | 36:1:1279:C:N3     | 2.55                     | 0.45              |
| 36:1:1246:G:H2'    | 36:1:1247:U:O4'    | 2.17                     | 0.45              |
| 36:1:1426:C:H4'    | 41:L4:40:THR:HB    | 1.99                     | 0.45              |
| 36:1:1493:G:C6     | 75:O9:13:MET:HE2   | 2.51                     | 0.45              |
| 36:1:2320:A:H2     | 79:Q3:16:VAL:HG13  | 1.81                     | 0.45              |
| 36:1:3046:A:H2'    | 36:1:3047:U:O4'    | 2.17                     | 0.45              |
| 36:1:3173:G:C2     | 69:O3:96:ALA:HB2   | 2.52                     | 0.45              |
| 86:1:4071:OHX:N1   | 86:1:4118:OHX:N4   | 2.65                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 86:1:4071:OHX:N3  | 86:1:4118:OHX:N6   | 2.64                     | 0.45              |
| 46:L9:7:GLU:OE2   | 46:L9:54:LYS:HE3   | 2.17                     | 0.45              |
| 46:L9:124:ARG:HG2 | 46:L9:164:ILE:HG13 | 1.99                     | 0.45              |
| 51:M5:58:GLY:HA3  | 51:M5:142:ILE:HD13 | 1.98                     | 0.45              |
| 55:M9:130:ASN:C   | 55:M9:132:PHE:N    | 2.75                     | 0.45              |
| 71:O5:49:LYS:HD2  | 71:O5:49:LYS:N     | 2.31                     | 0.45              |
| 1:6:416:A:H4'     | 1:6:417:A:OP2      | 2.16                     | 0.45              |
| 1:6:478:A:C2      | 1:6:511:A:C2       | 3.05                     | 0.45              |
| 1:6:1096:C:H6     | 1:6:1096:C:H2'     | 1.56                     | 0.45              |
| 1:6:1178:G:H4'    | 35:sM:83:LYS:CE    | 2.47                     | 0.45              |
| 1:6:1699:G:H2'    | 1:6:1700:C:H5'     | 1.97                     | 0.45              |
| 1:6:1772:C:OP1    | 77:q1:2:ARG:HD3    | 2.17                     | 0.45              |
| 3:s1:55:LYS:HD3   | 3:s1:55:LYS:HA     | 1.63                     | 0.45              |
| 4:s2:140:ARG:HD2  | 23:d1:10:GLU:OE1   | 2.16                     | 0.45              |
| 7:s5:43:PHE:N     | 7:s5:46:TRP:H      | 2.15                     | 0.45              |
| 7:s5:120:ILE:O    | 7:s5:124:LEU:HD13  | 2.16                     | 0.45              |
| 10:s8:66:SER:O    | 10:s8:183:ILE:HG23 | 2.17                     | 0.45              |
| 20:c8:52:VAL:HG13 | 20:c8:61:LEU:HD21  | 1.98                     | 0.45              |
| 24:d2:23:ARG:NH1  | 24:d2:66:ASN:HA    | 2.32                     | 0.45              |
| 28:d6:73:TYR:CE2  | 28:d6:83:ILE:HD12  | 2.52                     | 0.45              |
| 36:5:585:A:OP1    | 69:o3:70:LYS:HE2   | 2.16                     | 0.45              |
| 36:5:1181:U:H2'   | 52:m6:122:GLN:NE2  | 2.32                     | 0.45              |
| 36:5:1947:G:N2    | 36:5:2102:U:C2     | 2.85                     | 0.45              |
| 36:5:3216:G:OP2   | 69:o3:2:ALA:HB2    | 2.17                     | 0.45              |
| 86:5:4212:OHX:N4  | 86:5:4222:OHX:N6   | 2.64                     | 0.45              |
| 38:8:121:U:O2'    | 38:8:122:U:H5'     | 2.17                     | 0.45              |
| 43:l6:54:TYR:HA   | 43:l6:65:ILE:HD12  | 1.98                     | 0.45              |
| 48:m1:153:LYS:O   | 48:m1:153:LYS:HG2  | 2.09                     | 0.45              |
| 50:m4:47:ASP:C    | 50:m4:49:PRO:HD3   | 2.41                     | 0.45              |
| 54:m8:86:THR:HG22 | 54:m8:105:ARG:HB2  | 1.99                     | 0.45              |
| 73:o7:65:ARG:HG3  | 73:o7:65:ARG:HH11  | 1.82                     | 0.45              |
| 76:q0:114:LYS:HG2 | 76:q0:115:CYS:N    | 2.30                     | 0.45              |
| 1:2:494:U:O2'     | 1:2:495:C:O5'      | 2.32                     | 0.45              |
| 86:2:2076:OHX:N4  | 86:2:2163:OHX:N1   | 2.64                     | 0.45              |
| 86:2:2096:OHX:N6  | 86:2:2109:OHX:N2   | 2.65                     | 0.45              |
| 2:S0:11:PRO:O     | 2:S0:15:GLN:HG3    | 2.17                     | 0.45              |
| 4:S2:148:LEU:HA   | 23:D1:4:ASP:HB2    | 1.98                     | 0.45              |
| 5:S3:58:VAL:O     | 5:S3:66:ILE:HG12   | 2.17                     | 0.45              |
| 10:S8:8:ARG:CD    | 10:S8:21:PHE:HB3   | 2.45                     | 0.45              |
| 22:D0:87:HIS:HB3  | 22:D0:89:ARG:NH1   | 2.32                     | 0.45              |
| 28:D6:36:ILE:HD11 | 28:D6:83:ILE:HG22  | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:D6:84:VAL:HG22  | 28:D6:85:ARG:N     | 2.30                     | 0.45              |
| 28:D6:87:ARG:HB3   | 28:D6:91:ASP:HB2   | 1.99                     | 0.45              |
| 36:1:716:A:N6      | 64:N8:117:ARG:HG3  | 2.32                     | 0.45              |
| 36:1:938:C:OP1     | 36:1:963:G:H5'     | 2.17                     | 0.45              |
| 36:1:1758:G:H1     | 36:1:1767:C:H42    | 1.65                     | 0.45              |
| 36:1:3242:G:H2'    | 40:L3:154:TYR:CE1  | 2.52                     | 0.45              |
| 44:L7:158:LYS:CG   | 44:L7:159:GLN:H    | 2.28                     | 0.45              |
| 45:L8:214:LEU:HD12 | 45:L8:214:LEU:HA   | 1.81                     | 0.45              |
| 48:M1:106:ILE:O    | 48:M1:106:ILE:HG12 | 2.16                     | 0.45              |
| 49:M3:107:GLU:OE2  | 72:O6:18:THR:HG23  | 2.17                     | 0.45              |
| 54:M8:40:THR:C     | 54:M8:42:ALA:H     | 2.24                     | 0.45              |
| 62:N6:45:ILE:HD12  | 62:N6:119:ILE:HG23 | 1.99                     | 0.45              |
| 71:O5:78:LYS:HA    | 71:O5:81:ARG:CD    | 2.44                     | 0.45              |
| 72:O6:62:ARG:HH22  | 72:O6:98:ARG:NH1   | 2.14                     | 0.45              |
| 72:O6:97:SER:C     | 72:O6:99:ARG:H     | 2.25                     | 0.45              |
| 1:6:713:A:H2'      | 1:6:714:G:H5''     | 1.99                     | 0.45              |
| 1:6:1275:A:C2'     | 5:s3:141:LYS:HZ3   | 2.30                     | 0.45              |
| 1:6:1595:U:H3'     | 1:6:1596:C:O2      | 2.17                     | 0.45              |
| 3:s1:164:ILE:O     | 3:s1:168:ILE:HG13  | 2.16                     | 0.45              |
| 4:s2:37:PRO:HA     | 4:s2:65:GLU:OE1    | 2.17                     | 0.45              |
| 4:s2:140:ARG:NH2   | 4:s2:226:THR:OG1   | 2.50                     | 0.45              |
| 6:s4:160:VAL:HG13  | 6:s4:169:ILE:HG23  | 1.99                     | 0.45              |
| 8:s6:57:ASP:HA     | 8:s6:106:LEU:HA    | 1.99                     | 0.45              |
| 9:s7:9:LEU:HB3     | 9:s7:10:SER:H      | 1.59                     | 0.45              |
| 12:c0:6:GLU:O      | 12:c0:10:LYS:HD3   | 2.17                     | 0.45              |
| 26:d4:57:VAL:HB    | 26:d4:60:PHE:CE2   | 2.52                     | 0.45              |
| 34:sR:44:SER:O     | 34:sR:58:VAL:HG13  | 2.17                     | 0.45              |
| 35:sM:77:THR:O     | 35:sM:79:SER:N     | 2.50                     | 0.45              |
| 36:5:495:G:H2'     | 36:5:496:C:O4'     | 2.16                     | 0.45              |
| 36:5:807:A:H61     | 36:5:934:G:H22     | 1.64                     | 0.45              |
| 36:5:2882:U:H2'    | 36:5:2883:U:C6     | 2.52                     | 0.45              |
| 86:5:4000:OHX:N6   | 86:5:4190:OHX:N3   | 2.65                     | 0.45              |
| 86:5:4033:OHX:N1   | 86:5:4081:OHX:N4   | 2.64                     | 0.45              |
| 37:7:40:C:O2       | 48:m1:72:ARG:NH2   | 2.47                     | 0.45              |
| 45:l8:166:LEU:HD23 | 45:l8:166:LEU:HA   | 1.71                     | 0.45              |
| 46:l9:87:LYS:NZ    | 46:l9:191:LEU:HD21 | 2.32                     | 0.45              |
| 51:m5:70:ASN:HD21  | 51:m5:93:LYS:HE3   | 1.81                     | 0.45              |
| 68:o2:77:ALA:HB3   | 68:o2:81:ASP:OD2   | 2.16                     | 0.45              |
| 73:o7:14:LYS:HE2   | 75:o9:51:ILE:HG13  | 1.99                     | 0.45              |
| 73:o7:69:HIS:ND1   | 73:o7:72:ARG:NH2   | 2.65                     | 0.45              |
| 74:o8:59:ALA:O     | 74:o8:62:ALA:HB3   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:732:G:C6       | 86:2:2130:OHX:N3   | 2.85                     | 0.45              |
| 1:2:986:G:H2'      | 1:2:987:G:O4'      | 2.17                     | 0.45              |
| 1:2:1114:G:O2'     | 1:2:1130:G:O6      | 2.31                     | 0.45              |
| 1:2:1278:G:H2'     | 1:2:1279:C:O4'     | 2.17                     | 0.45              |
| 86:2:2116:OHX:N5   | 86:C1:201:OHX:N1   | 2.65                     | 0.45              |
| 2:S0:30:GLN:NE2    | 2:S0:149:LEU:HD13  | 2.32                     | 0.45              |
| 2:S0:61:ALA:HA     | 2:S0:64:ILE:HD12   | 1.99                     | 0.45              |
| 2:S0:103:THR:HA    | 2:S0:104:PRO:HD3   | 1.74                     | 0.45              |
| 3:S1:41:ARG:NH2    | 3:S1:97:LEU:HD11   | 2.32                     | 0.45              |
| 4:S2:165:VAL:HA    | 4:S2:201:ASN:O     | 2.17                     | 0.45              |
| 11:S9:143:ILE:HG22 | 11:S9:145:SER:H    | 1.82                     | 0.45              |
| 11:S9:171:ARG:NH1  | 11:S9:174:ARG:HG3  | 2.32                     | 0.45              |
| 12:C0:25:LYS:HD2   | 12:C0:59:PHE:CZ    | 2.51                     | 0.45              |
| 15:C3:99:ARG:O     | 15:C3:103:GLU:HG2  | 2.16                     | 0.45              |
| 16:C4:112:ILE:HB   | 28:D6:57:SER:OG    | 2.16                     | 0.45              |
| 17:C5:28:MET:O     | 17:C5:32:ASP:HB2   | 2.17                     | 0.45              |
| 19:C7:80:ARG:C     | 19:C7:82:ASP:H     | 2.24                     | 0.45              |
| 20:C8:35:ILE:HB    | 20:C8:38:VAL:HG21  | 1.99                     | 0.45              |
| 28:D6:23:CYS:CB    | 28:D6:74:CYS:HB3   | 2.45                     | 0.45              |
| 36:1:537:A:H2'     | 36:1:538:G:O4'     | 2.17                     | 0.45              |
| 36:1:701:G:H2'     | 36:1:702:C:C6      | 2.52                     | 0.45              |
| 36:1:1792:C:H2'    | 36:1:1795:U:C5     | 2.52                     | 0.45              |
| 36:1:1887:A:OP2    | 86:1:3896:OHX:N4   | 2.50                     | 0.45              |
| 36:1:3030:G:N7     | 86:1:4077:OHX:N6   | 2.65                     | 0.45              |
| 36:1:3174:A:OP1    | 69:O3:97:SER:OG    | 2.28                     | 0.45              |
| 36:1:3275:U:O4     | 69:O3:62:SER:OG    | 2.34                     | 0.45              |
| 36:1:3362:A:H2'    | 36:1:3363:U:O4'    | 2.17                     | 0.45              |
| 86:1:4071:OHX:N3   | 86:1:4118:OHX:N4   | 2.64                     | 0.45              |
| 86:1:4084:OHX:N2   | 86:1:4153:OHX:N5   | 2.65                     | 0.45              |
| 40:L3:168:LYS:O    | 40:L3:319:ASN:ND2  | 2.37                     | 0.45              |
| 40:L3:296:THR:HG22 | 40:L3:298:PHE:H    | 1.82                     | 0.45              |
| 40:L3:306:THR:HG22 | 40:L3:310:GLY:HA2  | 1.97                     | 0.45              |
| 41:L4:42:VAL:HG12  | 41:L4:236:LEU:HD21 | 1.98                     | 0.45              |
| 43:L6:89:THR:HG21  | 50:M4:115:PHE:HB2  | 1.98                     | 0.45              |
| 51:M5:91:GLU:C     | 51:M5:93:LYS:HE3   | 2.42                     | 0.45              |
| 63:N7:10:VAL:HB    | 63:N7:83:THR:CG2   | 2.46                     | 0.45              |
| 67:O1:19:ARG:HD3   | 67:O1:35:GLU:CG    | 2.47                     | 0.45              |
| 1:6:79:C:H4'       | 8:s6:173:PRO:O     | 2.17                     | 0.45              |
| 1:6:276:C:H1'      | 1:6:277:U:C5       | 2.52                     | 0.45              |
| 1:6:319:U:H1'      | 1:6:323:A:C4       | 2.52                     | 0.45              |
| 1:6:333:A:C6       | 1:6:334:G:C6       | 3.05                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:6:674:C:H2'     | 1:6:675:U:C6       | 2.51                     | 0.45              |
| 1:6:1007:C:H5''   | 16:c4:135:ARG:HG3  | 1.99                     | 0.45              |
| 1:6:1070:C:H4'    | 29:d7:17:ARG:HD3   | 1.99                     | 0.45              |
| 1:6:1552:U:O4     | 17:c5:40:ARG:NH2   | 2.39                     | 0.45              |
| 1:6:1567:U:C5     | 1:6:1568:C:C4      | 3.05                     | 0.45              |
| 1:6:1698:G:N2     | 1:6:1699:G:C8      | 2.85                     | 0.45              |
| 2:s0:90:ALA:HB1   | 2:s0:95:ALA:O      | 2.17                     | 0.45              |
| 4:s2:86:VAL:C     | 4:s2:87:GLN:HG2    | 2.42                     | 0.45              |
| 6:s4:26:CYS:HB2   | 6:s4:27:TYR:CE2    | 2.52                     | 0.45              |
| 7:s5:59:VAL:HG12  | 7:s5:60:ASP:H      | 1.82                     | 0.45              |
| 9:s7:44:LYS:HE2   | 9:s7:44:LYS:HB3    | 1.83                     | 0.45              |
| 12:c0:1:MET:HE2   | 12:c0:41:TYR:CE1   | 2.51                     | 0.45              |
| 13:c1:86:ILE:HD13 | 13:c1:86:ILE:HG21  | 1.51                     | 0.45              |
| 36:5:240:U:O2'    | 36:5:241:G:H8      | 2.00                     | 0.45              |
| 36:5:283:G:O6     | 36:5:304:G:H1'     | 2.17                     | 0.45              |
| 36:5:1076:C:H4'   | 65:n9:38:LYS:HD2   | 1.99                     | 0.45              |
| 36:5:1655:G:C5'   | 36:5:1655:G:C8     | 3.00                     | 0.45              |
| 86:5:4054:OHX:N4  | 86:5:4108:OHX:N1   | 2.65                     | 0.45              |
| 38:8:157:U:H2'    | 38:8:158:U:C6      | 2.52                     | 0.45              |
| 39:l2:44:ILE:HG23 | 39:l2:87:PHE:CE1   | 2.52                     | 0.45              |
| 40:l3:81:THR:HB   | 40:l3:321:PHE:HA   | 1.99                     | 0.45              |
| 44:l7:96:PRO:HG2  | 44:l7:99:PRO:HG2   | 1.97                     | 0.45              |
| 47:m0:152:LEU:HA  | 47:m0:152:LEU:HD23 | 1.66                     | 0.45              |
| 62:n6:108:LYS:HD3 | 62:n6:108:LYS:HA   | 1.61                     | 0.45              |
| 63:n7:99:GLU:HG3  | 63:n7:100:THR:N    | 2.32                     | 0.45              |
| 67:o1:85:ALA:O    | 67:o1:86:LYS:C     | 2.60                     | 0.45              |
| 70:o4:8:ARG:HB2   | 70:o4:34:HIS:CD2   | 2.52                     | 0.45              |
| 82:p0:25:LEU:HD12 | 82:p0:26:PHE:N     | 2.32                     | 0.45              |
| 82:p0:77:LEU:HA   | 82:p0:80:VAL:HG12  | 1.98                     | 0.45              |
| 1:2:549:G:C2      | 1:2:550:A:C8       | 3.05                     | 0.44              |
| 1:2:929:A:N6      | 1:2:930:A:C6       | 2.85                     | 0.44              |
| 1:2:1492:A:O2'    | 1:2:1493:A:H8      | 1.99                     | 0.44              |
| 4:S2:139:ILE:HD12 | 4:S2:191:ALA:HB1   | 1.99                     | 0.44              |
| 6:S4:126:VAL:HG13 | 6:S4:158:ASP:O     | 2.18                     | 0.44              |
| 11:S9:93:LEU:HA   | 11:S9:96:VAL:CG1   | 2.38                     | 0.44              |
| 18:C6:127:LYS:HA  | 18:C6:134:ALA:HA   | 1.99                     | 0.44              |
| 26:D4:104:SER:HB3 | 26:D4:107:GLN:CG   | 2.47                     | 0.44              |
| 33:E1:126:CYS:HB3 | 33:E1:130:VAL:HG21 | 1.99                     | 0.44              |
| 34:SR:216:LYS:HA  | 34:SR:239:GLU:HG3  | 1.99                     | 0.44              |
| 36:1:378:A:N7     | 36:1:391:A:H2      | 2.15                     | 0.44              |
| 36:1:422:A:C2     | 36:1:2363:A:H4'    | 2.53                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1109:U:H2'    | 36:1:1110:U:O4'    | 2.17                     | 0.44              |
| 36:1:2206:G:C2     | 36:1:2207:A:C8     | 3.05                     | 0.44              |
| 36:1:2403:G:C2     | 36:1:2404:A:N7     | 2.83                     | 0.44              |
| 38:4:37:A:H5''     | 38:4:39:G:O4'      | 2.17                     | 0.44              |
| 42:L5:184:ASP:HB3  | 42:L5:187:THR:HG23 | 1.98                     | 0.44              |
| 44:L7:151:ARG:HD2  | 44:L7:244:ASN:ND2  | 2.32                     | 0.44              |
| 48:M1:63:GLU:O     | 48:M1:64:LYS:HB2   | 2.16                     | 0.44              |
| 51:M5:143:ARG:HH21 | 71:O5:92:LEU:HD23  | 1.82                     | 0.44              |
| 55:M9:99:LEU:O     | 55:M9:103:ARG:HB2  | 2.17                     | 0.44              |
| 57:N1:88:ARG:NH2   | 65:N9:33:LYS:HB3   | 2.32                     | 0.44              |
| 62:N6:52:ARG:C     | 62:N6:54:ASP:H     | 2.25                     | 0.44              |
| 64:N8:75:LEU:O     | 64:N8:76:ASP:C     | 2.60                     | 0.44              |
| 67:O1:5:LYS:HA     | 67:O1:89:LEU:HD21  | 1.99                     | 0.44              |
| 1:6:1591:C:H2'     | 1:6:1592:A:C8      | 2.52                     | 0.44              |
| 2:s0:22:THR:HA     | 2:s0:169:SER:OG    | 2.17                     | 0.44              |
| 6:s4:180:LEU:N     | 6:s4:229:GLY:O     | 2.47                     | 0.44              |
| 10:s8:31:ARG:HH21  | 10:s8:48:THR:HG22  | 1.83                     | 0.44              |
| 17:c5:77:ARG:HB3   | 17:c5:102:PHE:CE1  | 2.52                     | 0.44              |
| 18:c6:127:LYS:HE2  | 18:c6:132:LYS:O    | 2.16                     | 0.44              |
| 20:c8:13:HIS:O     | 20:c8:14:ILE:HG22  | 2.17                     | 0.44              |
| 25:d3:130:VAL:O    | 25:d3:131:SER:CB   | 2.62                     | 0.44              |
| 36:5:144:A:N6      | 36:5:145:G:C2      | 2.85                     | 0.44              |
| 36:5:2191:U:H2'    | 36:5:2192:C:O4'    | 2.17                     | 0.44              |
| 36:5:2437:G:H2'    | 36:5:2438:A:O4'    | 2.17                     | 0.44              |
| 36:5:2510:U:O2'    | 36:5:2511:A:H5''   | 2.16                     | 0.44              |
| 36:5:2947:G:OP2    | 36:5:2947:G:H4'    | 2.17                     | 0.44              |
| 36:5:3149:G:O2'    | 40:l3:129:ALA:O    | 2.30                     | 0.44              |
| 36:5:3291:G:H2'    | 36:5:3292:A:C8     | 2.52                     | 0.44              |
| 37:7:58:C:OP1      | 86:7:217:OHX:N3    | 2.51                     | 0.44              |
| 42:l5:98:ALA:O     | 42:l5:162:ALA:HA   | 2.17                     | 0.44              |
| 42:l5:110:LEU:C    | 42:l5:110:LEU:HD23 | 2.43                     | 0.44              |
| 42:l5:270:LYS:O    | 42:l5:273:ARG:HD2  | 2.17                     | 0.44              |
| 45:l8:116:VAL:C    | 45:l8:118:GLU:N    | 2.74                     | 0.44              |
| 55:m9:106:LEU:HD12 | 55:m9:106:LEU:HA   | 1.80                     | 0.44              |
| 55:m9:109:TYR:HB3  | 55:m9:115:ILE:HG12 | 1.99                     | 0.44              |
| 57:n1:73:GLY:HA2   | 57:n1:89:LEU:O     | 2.17                     | 0.44              |
| 60:n4:122:ALA:O    | 60:n4:125:ALA:HB3  | 2.18                     | 0.44              |
| 1:2:489:C:H2'      | 1:2:490:C:C6       | 2.52                     | 0.44              |
| 1:2:603:U:H2'      | 1:2:604:A:H8       | 1.82                     | 0.44              |
| 1:2:755:A:HO2'     | 1:2:756:A:P        | 2.40                     | 0.44              |
| 1:2:1067:C:H2'     | 1:2:1068:C:C6      | 2.48                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:1113:A:H4'    | 1:2:1114:G:OP1     | 2.17                     | 0.44              |
| 86:2:2096:OHX:N4  | 86:2:2109:OHX:N1   | 2.65                     | 0.44              |
| 2:S0:57:LEU:HG    | 2:S0:177:LEU:HD23  | 1.99                     | 0.44              |
| 2:S0:172:LEU:HD22 | 2:S0:176:LEU:HG    | 1.98                     | 0.44              |
| 4:S2:65:GLU:O     | 4:S2:68:ILE:HB     | 2.17                     | 0.44              |
| 5:S3:64:ARG:O     | 5:S3:67:ASN:HB2    | 2.16                     | 0.44              |
| 6:S4:72:VAL:HG23  | 6:S4:77:ARG:HB2    | 1.98                     | 0.44              |
| 6:S4:87:MET:SD    | 6:S4:123:LEU:HB2   | 2.58                     | 0.44              |
| 9:S7:60:ILE:HD12  | 9:S7:92:PHE:CE2    | 2.53                     | 0.44              |
| 15:C3:28:LEU:HB3  | 15:C3:29:SER:H     | 1.58                     | 0.44              |
| 18:C6:38:LEU:C    | 18:C6:40:GLU:H     | 2.23                     | 0.44              |
| 24:D2:6:VAL:HG22  | 24:D2:29:PRO:HD2   | 1.99                     | 0.44              |
| 36:1:412:G:OP1    | 53:M7:62:ARG:NH1   | 2.50                     | 0.44              |
| 36:1:1722:U:H1'   | 55:M9:96:ILE:HG12  | 1.98                     | 0.44              |
| 36:1:2443:A:N6    | 36:1:2503:G:C2     | 2.86                     | 0.44              |
| 36:1:2662:G:H2'   | 36:1:2663:G:H8     | 1.82                     | 0.44              |
| 36:1:2679:A:HO2'  | 48:M1:52:TYR:HH    | 1.61                     | 0.44              |
| 36:1:3095:U:H2'   | 36:1:3096:C:H6     | 1.81                     | 0.44              |
| 36:1:3222:U:H6    | 36:1:3222:U:H5''   | 1.81                     | 0.44              |
| 39:L2:77:ILE:CD1  | 39:L2:128:ARG:HB3  | 2.48                     | 0.44              |
| 40:L3:296:THR:HB  | 40:L3:299:ASP:HB2  | 1.99                     | 0.44              |
| 45:L8:78:PHE:CD2  | 45:L8:179:ILE:HD13 | 2.52                     | 0.44              |
| 47:M0:9:TYR:CG    | 47:M0:97:LEU:HD13  | 2.52                     | 0.44              |
| 48:M1:23:VAL:HG11 | 48:M1:29:ARG:HG2   | 1.99                     | 0.44              |
| 50:M4:20:VAL:HG22 | 50:M4:66:THR:OG1   | 2.17                     | 0.44              |
| 64:N8:74:ASN:CB   | 64:N8:76:ASP:HB2   | 2.46                     | 0.44              |
| 68:O2:20:HIS:CG   | 68:O2:42:VAL:HG21  | 2.52                     | 0.44              |
| 68:O2:64:LYS:HE2  | 68:O2:65:PHE:CZ    | 2.52                     | 0.44              |
| 1:6:542:A:N7      | 1:6:543:C:H2'      | 2.32                     | 0.44              |
| 1:6:594:A:H4'     | 1:6:595:G:H5'      | 1.98                     | 0.44              |
| 2:s0:198:MET:HE1  | 19:c7:88:VAL:HB    | 1.99                     | 0.44              |
| 3:s1:133:TYR:CZ   | 3:s1:181:LEU:HD12  | 2.52                     | 0.44              |
| 6:s4:49:ARG:HG3   | 6:s4:50:ASN:N      | 2.28                     | 0.44              |
| 7:s5:61:TYR:HD2   | 7:s5:164:PRO:HB2   | 1.82                     | 0.44              |
| 14:c2:125:ASN:ND2 | 35:sM:169:ALA:H    | 2.15                     | 0.44              |
| 16:c4:102:LEU:CD1 | 28:d6:45:VAL:HG12  | 2.47                     | 0.44              |
| 18:c6:82:ARG:NH1  | 18:c6:114:ARG:HB2  | 2.31                     | 0.44              |
| 29:d7:59:CYS:O    | 29:d7:61:THR:N     | 2.50                     | 0.44              |
| 36:5:92:G:H5'     | 36:5:93:C:C5'      | 2.45                     | 0.44              |
| 36:5:1313:G:H5'   | 52:m6:83:ALA:HB1   | 2.00                     | 0.44              |
| 36:5:1880:U:H2'   | 36:5:1881:A:O4'    | 2.16                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:8:109:A:C2'     | 38:8:110:C:H5'     | 2.47                     | 0.44              |
| 39:12:52:SER:HB3   | 39:12:191:LEU:HD12 | 1.99                     | 0.44              |
| 41:14:22:LEU:HA    | 41:14:23:PRO:HD3   | 1.69                     | 0.44              |
| 41:14:209:TYR:O    | 41:14:230:VAL:HG22 | 2.18                     | 0.44              |
| 42:15:194:LEU:HD23 | 42:15:194:LEU:HA   | 1.83                     | 0.44              |
| 42:15:268:GLU:C    | 42:15:270:LYS:H    | 2.26                     | 0.44              |
| 51:m5:8:GLU:HG3    | 51:m5:50:ARG:NH1   | 2.32                     | 0.44              |
| 63:n7:80:LEU:O     | 63:n7:82:PRO:HD3   | 2.17                     | 0.44              |
| 70:o4:3:GLN:CD     | 70:o4:30:LEU:HB2   | 2.43                     | 0.44              |
| 73:o7:63:ARG:O     | 73:o7:68:LYS:HE3   | 2.17                     | 0.44              |
| 1:2:350:U:O2       | 1:2:352:A:C6       | 2.70                     | 0.44              |
| 1:2:1236:A:O4'     | 33:E1:138:ARG:NH2  | 2.50                     | 0.44              |
| 1:2:1459:C:N4      | 20:C8:139:LYS:HE2  | 2.31                     | 0.44              |
| 2:S0:13:ASP:HA     | 2:S0:16:LEU:HD12   | 1.99                     | 0.44              |
| 4:S2:81:MET:HE1    | 4:S2:186:LYS:HB3   | 1.99                     | 0.44              |
| 6:S4:71:LYS:HB3    | 6:S4:76:VAL:HA     | 2.00                     | 0.44              |
| 7:S5:31:GLU:O      | 7:S5:35:GLN:HB2    | 2.16                     | 0.44              |
| 14:C2:38:HIS:O     | 14:C2:125:ASN:ND2  | 2.50                     | 0.44              |
| 14:C2:59:LEU:HA    | 14:C2:87:PRO:HB2   | 2.00                     | 0.44              |
| 21:C9:132:LEU:O    | 21:C9:135:ILE:HG13 | 2.17                     | 0.44              |
| 22:D0:22:ILE:HD12  | 22:D0:118:VAL:HA   | 1.98                     | 0.44              |
| 23:D1:74:GLN:HB2   | 23:D1:79:LEU:HB2   | 1.99                     | 0.44              |
| 30:D8:18:ARG:HD3   | 30:D8:25:VAL:O     | 2.17                     | 0.44              |
| 31:D9:54:LYS:HE3   | 31:D9:54:LYS:HB3   | 1.72                     | 0.44              |
| 36:1:149:U:OP2     | 51:M5:49:ARG:NH2   | 2.48                     | 0.44              |
| 36:1:716:A:C6      | 64:N8:117:ARG:HG3  | 2.53                     | 0.44              |
| 36:1:736:A:H2'     | 36:1:737:G:O4'     | 2.16                     | 0.44              |
| 36:1:1062:A:N3     | 57:N1:130:ARG:NH2  | 2.58                     | 0.44              |
| 36:1:1580:A:H5'    | 36:1:2522:G:C5     | 2.53                     | 0.44              |
| 36:1:1591:G:H5''   | 70:O4:37:LYS:NZ    | 2.32                     | 0.44              |
| 36:1:2303:A:P      | 77:Q1:23:ARG:NH2   | 2.90                     | 0.44              |
| 36:1:3019:U:O4     | 86:1:3993:OHX:N4   | 2.51                     | 0.44              |
| 86:1:4065:OHX:N3   | 86:1:4177:OHX:N5   | 2.65                     | 0.44              |
| 86:3:218:OHX:N2    | 86:3:223:OHX:N5    | 2.65                     | 0.44              |
| 39:L2:179:LEU:O    | 39:L2:180:LEU:HB2  | 2.17                     | 0.44              |
| 40:L3:55:THR:O     | 40:L3:56:ILE:HD12  | 2.16                     | 0.44              |
| 42:L5:261:THR:OG1  | 42:L5:264:GLN:HG3  | 2.17                     | 0.44              |
| 45:L8:130:TYR:HD1  | 45:L8:202:GLU:HB3  | 1.82                     | 0.44              |
| 46:L9:75:VAL:HA    | 46:L9:78:MET:HE2   | 1.99                     | 0.44              |
| 53:M7:39:TRP:O     | 53:M7:114:VAL:HG12 | 2.17                     | 0.44              |
| 56:N0:77:VAL:HG21  | 56:N0:94:ILE:HD12  | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:N2:33:TYR:HE2   | 58:N2:63:VAL:HG21  | 1.80                     | 0.44              |
| 1:6:542:A:OP1      | 1:6:544:A:C5       | 2.71                     | 0.44              |
| 1:6:934:C:C6       | 28:d6:11:ASN:HB3   | 2.52                     | 0.44              |
| 1:6:1540:G:C6      | 1:6:1541:G:C4      | 3.05                     | 0.44              |
| 2:s0:13:ASP:CG     | 2:s0:179:ARG:HH22  | 2.26                     | 0.44              |
| 2:s0:69:ASN:HB3    | 2:s0:71:GLU:OE1    | 2.17                     | 0.44              |
| 4:s2:188:LEU:HD23  | 4:s2:188:LEU:HA    | 1.87                     | 0.44              |
| 11:s9:78:ARG:HG3   | 11:s9:79:ARG:N     | 2.32                     | 0.44              |
| 12:c0:2:LEU:HB3    | 12:c0:3:MET:H      | 1.56                     | 0.44              |
| 15:c3:114:ARG:HG2  | 15:c3:114:ARG:NH1  | 2.17                     | 0.44              |
| 20:c8:28:ILE:HG13  | 20:c8:56:LYS:O     | 2.17                     | 0.44              |
| 34:sR:206:PRO:HG2  | 34:sR:247:PRO:HA   | 1.98                     | 0.44              |
| 36:5:72:C:C2       | 36:5:74:G:H1'      | 2.53                     | 0.44              |
| 36:5:685:G:OP1     | 49:m3:35:ARG:NH1   | 2.50                     | 0.44              |
| 36:5:1048:A:H2'    | 47:m0:22:TYR:CZ    | 2.53                     | 0.44              |
| 36:5:1715:A:H4'    | 36:5:1716:U:OP1    | 2.18                     | 0.44              |
| 36:5:2161:G:O3'    | 39:l2:227:ARG:NH2  | 2.50                     | 0.44              |
| 36:5:2426:U:H2'    | 36:5:2427:U:C6     | 2.53                     | 0.44              |
| 36:5:3384:U:H2'    | 36:5:3385:U:C6     | 2.52                     | 0.44              |
| 37:7:113:C:C4      | 37:7:114:U:C4      | 3.06                     | 0.44              |
| 86:7:219:OHX:N5    | 86:7:224:OHX:N6    | 2.66                     | 0.44              |
| 38:8:104:A:C8      | 38:8:105:A:C8      | 3.05                     | 0.44              |
| 39:l2:96:LEU:O     | 79:q3:87:ARG:HD3   | 2.17                     | 0.44              |
| 40:l3:335:ILE:HG13 | 40:l3:336:VAL:N    | 2.32                     | 0.44              |
| 47:m0:19:LYS:HG3   | 47:m0:26:VAL:CG2   | 2.47                     | 0.44              |
| 61:n5:132:ALA:HA   | 61:n5:135:ILE:HG22 | 1.99                     | 0.44              |
| 62:n6:52:ARG:O     | 62:n6:53:ASP:HB2   | 2.17                     | 0.44              |
| 69:o3:90:PRO:O     | 69:o3:91:ALA:HB3   | 2.17                     | 0.44              |
| 71:o5:21:LEU:HD22  | 71:o5:25:LYS:HE3   | 1.99                     | 0.44              |
| 79:q3:80:ARG:HE    | 79:q3:80:ARG:HB2   | 1.39                     | 0.44              |
| 82:p0:105:VAL:HG23 | 82:p0:184:GLY:HA3  | 1.98                     | 0.44              |
| 1:2:646:C:H2'      | 1:2:647:G:C8       | 2.53                     | 0.44              |
| 1:2:1301:U:H2'     | 1:2:1302:U:O4'     | 2.17                     | 0.44              |
| 1:2:1422:A:C2      | 1:2:1423:U:C2      | 3.05                     | 0.44              |
| 1:2:1511:U:H2'     | 1:2:1512:G:C8      | 2.52                     | 0.44              |
| 6:S4:45:ILE:HA     | 6:S4:61:VAL:HG11   | 1.99                     | 0.44              |
| 8:S6:141:ILE:HG21  | 8:S6:153:VAL:HG13  | 1.99                     | 0.44              |
| 12:C0:8:ARG:HD2    | 12:C0:12:HIS:CE1   | 2.52                     | 0.44              |
| 25:D3:69:ARG:HH11  | 25:D3:116:ASP:CG   | 2.24                     | 0.44              |
| 29:D7:74:SER:O     | 29:D7:76:GLY:N     | 2.50                     | 0.44              |
| 36:1:374:A:N3      | 36:1:376:G:H5''    | 2.31                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:980:A:H2'     | 36:1:981:U:C1'     | 2.47                     | 0.44              |
| 36:1:2098:C:H2'    | 36:1:2099:A:C8     | 2.43                     | 0.44              |
| 36:1:2191:U:H2'    | 36:1:2192:C:O4'    | 2.18                     | 0.44              |
| 36:1:2358:A:H2'    | 36:1:2359:C:O4'    | 2.18                     | 0.44              |
| 36:1:2366:C:OP1    | 40:L3:259:HIS:NE2  | 2.43                     | 0.44              |
| 36:1:2712:U:H2'    | 36:1:2713:U:C6     | 2.52                     | 0.44              |
| 36:1:2771:U:H4'    | 78:Q2:15:LYS:NZ    | 2.32                     | 0.44              |
| 36:1:3006:A:C2     | 36:1:3141:A:C4     | 3.05                     | 0.44              |
| 36:1:3066:U:H2'    | 36:1:3067:C:C6     | 2.53                     | 0.44              |
| 40:L3:290:ASP:C    | 40:L3:291:GLU:O    | 2.60                     | 0.44              |
| 44:L7:87:VAL:HG11  | 44:L7:243:MET:HE1  | 2.00                     | 0.44              |
| 47:M0:99:ILE:HG22  | 47:M0:123:HIS:HB2  | 1.99                     | 0.44              |
| 49:M3:122:LYS:HA   | 71:O5:120:ALA:HA   | 2.00                     | 0.44              |
| 51:M5:75:VAL:HA    | 51:M5:76:PRO:HD3   | 1.75                     | 0.44              |
| 54:M8:162:ALA:HA   | 54:M8:163:PRO:HD2  | 1.53                     | 0.44              |
| 63:N7:17:ARG:O     | 63:N7:19:ALA:N     | 2.51                     | 0.44              |
| 66:O0:42:ILE:HD11  | 66:O0:67:VAL:HG22  | 1.99                     | 0.44              |
| 1:6:82:U:H2'       | 1:6:83:G:O4'       | 2.18                     | 0.44              |
| 1:6:1796:C:C5      | 28:d6:6:ALA:N      | 2.84                     | 0.44              |
| 2:s0:59:LEU:HD12   | 23:d1:79:LEU:HD21  | 1.98                     | 0.44              |
| 6:s4:77:ARG:HH11   | 6:s4:77:ARG:HG3    | 1.82                     | 0.44              |
| 9:s7:110:GLN:HE21  | 9:s7:110:GLN:HB3   | 1.56                     | 0.44              |
| 10:s8:49:ARG:O     | 10:s8:52:ASN:ND2   | 2.50                     | 0.44              |
| 14:c2:95:LYS:HA    | 14:c2:117:GLY:HA2  | 2.00                     | 0.44              |
| 18:c6:57:LEU:HD12  | 18:c6:57:LEU:H     | 1.83                     | 0.44              |
| 27:d5:82:HIS:C     | 27:d5:84:GLU:H     | 2.26                     | 0.44              |
| 33:e1:86:THR:HG23  | 33:e1:87:THR:H     | 1.82                     | 0.44              |
| 34:sR:133:VAL:HG12 | 34:sR:141:LEU:HD12 | 1.98                     | 0.44              |
| 36:5:284:A:H4'     | 36:5:285:A:N3      | 2.33                     | 0.44              |
| 36:5:353:G:O6      | 73:o7:55:ARG:NH1   | 2.51                     | 0.44              |
| 36:5:1046:A:H2'    | 36:5:1049:C:C5     | 2.52                     | 0.44              |
| 36:5:2115:G:H22    | 36:5:2120:A:H1'    | 1.83                     | 0.44              |
| 36:5:2767:U:O3'    | 78:q2:31:GLY:HA3   | 2.17                     | 0.44              |
| 42:l5:76:ALA:CB    | 42:l5:109:THR:HG22 | 2.47                     | 0.44              |
| 59:n3:74:MET:HB3   | 59:n3:74:MET:HE2   | 1.61                     | 0.44              |
| 59:n3:93:LEU:HD23  | 59:n3:93:LEU:H     | 1.81                     | 0.44              |
| 69:o3:91:ALA:C     | 69:o3:93:THR:N     | 2.75                     | 0.44              |
| 1:2:25:C:H6        | 1:2:25:C:H2'       | 1.66                     | 0.44              |
| 1:2:591:A:H2'      | 1:2:592:A:H8       | 1.82                     | 0.44              |
| 1:2:751:G:H2'      | 1:2:752:A:H8       | 1.83                     | 0.44              |
| 1:2:975:C:H5''     | 15:C3:109:LYS:HE3  | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1498:G:C2'     | 1:2:1499:G:H5'     | 2.47                     | 0.44              |
| 1:2:1557:U:OP2     | 1:2:1559:A:O2'     | 2.18                     | 0.44              |
| 1:2:1595:U:N3      | 1:2:1600:A:C2      | 2.81                     | 0.44              |
| 3:S1:35:PRO:HB2    | 3:S1:36:SER:H      | 1.52                     | 0.44              |
| 4:S2:82:ASN:OD1    | 4:S2:83:ILE:N      | 2.50                     | 0.44              |
| 4:S2:123:GLY:HA2   | 4:S2:126:ARG:NH1   | 2.33                     | 0.44              |
| 5:S3:18:TYR:CE1    | 5:S3:37:VAL:HG23   | 2.52                     | 0.44              |
| 6:S4:13:ALA:O      | 6:S4:39:ARG:NH2    | 2.51                     | 0.44              |
| 6:S4:18:TRP:HE3    | 6:S4:20:LEU:HD11   | 1.83                     | 0.44              |
| 6:S4:61:VAL:HG12   | 6:S4:65:LEU:HD12   | 1.98                     | 0.44              |
| 6:S4:131:LEU:HD22  | 6:S4:131:LEU:HA    | 1.82                     | 0.44              |
| 11:S9:31:ALA:HA    | 11:S9:36:LEU:HD12  | 2.00                     | 0.44              |
| 11:S9:157:ASP:OD2  | 11:S9:158:PHE:N    | 2.51                     | 0.44              |
| 17:C5:28:MET:HE2   | 17:C5:28:MET:HB3   | 1.71                     | 0.44              |
| 22:D0:37:VAL:O     | 22:D0:41:ILE:HD13  | 2.17                     | 0.44              |
| 27:D5:43:ASP:HB2   | 27:D5:46:LYS:HG3   | 1.98                     | 0.44              |
| 36:1:269:G:H5'     | 51:M5:120:TRP:CE3  | 2.52                     | 0.44              |
| 36:1:1035:G:H3'    | 36:1:1036:A:H8     | 1.83                     | 0.44              |
| 36:1:1127:G:H8     | 36:1:1127:G:O5'    | 2.00                     | 0.44              |
| 36:1:1556:C:H2'    | 36:1:2169:G:N2     | 2.32                     | 0.44              |
| 36:1:2282:U:O2     | 36:1:2310:U:H4'    | 2.16                     | 0.44              |
| 36:1:2971:A:H3'    | 36:1:2971:A:N3     | 2.33                     | 0.44              |
| 86:1:4023:OHX:N3   | 86:1:4061:OHX:N5   | 2.65                     | 0.44              |
| 38:4:141:C:OP1     | 51:M5:109:ARG:NH1  | 2.49                     | 0.44              |
| 39:L2:5:ILE:HG22   | 39:L2:208:ASP:O    | 2.16                     | 0.44              |
| 40:L3:121:ASN:O    | 40:L3:125:SER:HB3  | 2.18                     | 0.44              |
| 40:L3:305:ILE:HG12 | 40:L3:321:PHE:CZ   | 2.52                     | 0.44              |
| 43:L6:5:LYS:O      | 43:L6:6:ALA:HB2    | 2.16                     | 0.44              |
| 49:M3:57:VAL:HG13  | 49:M3:147:ILE:CG2  | 2.47                     | 0.44              |
| 50:M4:45:LEU:HD12  | 50:M4:56:GLN:O     | 2.17                     | 0.44              |
| 51:M5:150:TRP:CZ3  | 51:M5:151:ILE:HG12 | 2.53                     | 0.44              |
| 53:M7:116:HIS:HB3  | 53:M7:149:VAL:HB   | 2.00                     | 0.44              |
| 59:N3:62:VAL:CG2   | 59:N3:74:MET:HE1   | 2.47                     | 0.44              |
| 60:N4:1:MET:HE3    | 60:N4:15:PRO:HD3   | 1.98                     | 0.44              |
| 62:N6:3:LYS:HD2    | 62:N6:8:VAL:HG22   | 1.99                     | 0.44              |
| 74:O8:36:LYS:HG2   | 74:O8:37:PRO:HD2   | 2.00                     | 0.44              |
| 1:6:137:U:H6       | 1:6:137:U:H2'      | 1.49                     | 0.44              |
| 1:6:231:U:H2'      | 1:6:232:U:H5''     | 1.99                     | 0.44              |
| 1:6:542:A:C8       | 1:6:543:C:H5'      | 2.51                     | 0.44              |
| 1:6:1039:A:O2'     | 1:6:1040:G:OP2     | 2.30                     | 0.44              |
| 1:6:1340:U:O4      | 18:c6:9:THR:HA     | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:6:1398:U:H4'    | 1:6:1399:C:OP2    | 2.16                     | 0.44              |
| 2:s0:55:GLU:OE2   | 23:d1:80:LYS:N    | 2.45                     | 0.44              |
| 3:s1:146:GLN:O    | 3:s1:147:ALA:C    | 2.60                     | 0.44              |
| 6:s4:45:ILE:HB    | 6:s4:80:THR:HG23  | 1.99                     | 0.44              |
| 7:s5:43:PHE:CE2   | 7:s5:90:ILE:HG21  | 2.52                     | 0.44              |
| 7:s5:161:ASP:O    | 30:d8:44:VAL:HA   | 2.18                     | 0.44              |
| 17:c5:12:PHE:CE2  | 48:m1:85:LYS:HE2  | 2.53                     | 0.44              |
| 27:d5:74:SER:HA   | 27:d5:77:ARG:NH2  | 2.32                     | 0.44              |
| 28:d6:10:ARG:HD3  | 28:d6:34:LYS:HA   | 1.98                     | 0.44              |
| 31:d9:6:VAL:O     | 31:d9:8:PHE:N     | 2.50                     | 0.44              |
| 33:e1:88:PRO:HA   | 33:e1:89:LYS:HA   | 1.55                     | 0.44              |
| 34:sR:16:HIS:O    | 34:sR:308:ASN:HB3 | 2.18                     | 0.44              |
| 36:5:83:U:OP2     | 86:5:4205:OHX:N4  | 2.51                     | 0.44              |
| 36:5:249:U:OP2    | 36:5:249:U:H2'    | 2.18                     | 0.44              |
| 36:5:420:G:O5'    | 36:5:420:G:OP1    | 2.35                     | 0.44              |
| 36:5:929:A:H2'    | 36:5:930:U:C6     | 2.53                     | 0.44              |
| 36:5:986:U:OP2    | 86:5:4146:OHX:N2  | 2.51                     | 0.44              |
| 36:5:1029:G:H2'   | 36:5:1030:A:H8    | 1.82                     | 0.44              |
| 36:5:1409:G:O6    | 86:5:4160:OHX:N6  | 2.51                     | 0.44              |
| 36:5:1815:U:O2'   | 36:5:1816:A:P     | 2.75                     | 0.44              |
| 36:5:2846:U:O2'   | 86:5:4052:OHX:N1  | 2.51                     | 0.44              |
| 36:5:3185:U:O2'   | 56:n0:170:THR:OG1 | 2.29                     | 0.44              |
| 86:5:4001:OHX:N4  | 86:5:4090:OHX:N1  | 2.66                     | 0.44              |
| 86:5:4001:OHX:N3  | 86:5:4090:OHX:N1  | 2.66                     | 0.44              |
| 86:5:4127:OHX:N4  | 86:5:4144:OHX:N2  | 2.66                     | 0.44              |
| 37:7:110:G:C6     | 37:7:111:U:C4     | 3.06                     | 0.44              |
| 86:7:219:OHX:N3   | 86:7:224:OHX:N4   | 2.66                     | 0.44              |
| 38:8:46:G:O2'     | 38:8:61:A:N1      | 2.43                     | 0.44              |
| 40:l3:40:PRO:C    | 40:l3:185:GLY:HA3 | 2.42                     | 0.44              |
| 42:l5:160:PHE:HA  | 42:l5:163:LEU:HB3 | 1.99                     | 0.44              |
| 43:l6:15:VAL:HG23 | 68:o2:5:PRO:HG2   | 2.00                     | 0.44              |
| 45:l8:177:TYR:CZ  | 45:l8:222:PHE:O   | 2.71                     | 0.44              |
| 81:m2:16:UNK:O    | 81:m2:61:UNK:N    | 2.50                     | 0.44              |
| 57:n1:14:MET:HE2  | 57:n1:15:PHE:CE2  | 2.52                     | 0.44              |
| 70:o4:65:VAL:HG12 | 70:o4:70:LYS:HE2  | 1.98                     | 0.44              |
| 71:o5:45:LYS:HZ3  | 71:o5:45:LYS:HG2  | 1.73                     | 0.44              |
| 1:2:73:U:H4'      | 1:2:74:U:OP1      | 2.18                     | 0.44              |
| 1:2:283:U:H5''    | 8:S6:188:ARG:HD3  | 1.99                     | 0.44              |
| 1:2:287:G:O2'     | 1:2:288:A:P       | 2.75                     | 0.44              |
| 1:2:417:A:H4'     | 1:2:418:G:O5'     | 2.16                     | 0.44              |
| 1:2:1393:C:H2'    | 1:2:1394:G:O4'    | 2.17                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1445:G:C5      | 33:E1:91:ILE:HB    | 2.53                     | 0.44              |
| 1:2:1537:C:N4      | 86:2:2155:OHX:N6   | 2.66                     | 0.44              |
| 1:2:1769:U:O2      | 16:C4:136:ARG:HD2  | 2.17                     | 0.44              |
| 86:2:2116:OHX:N2   | 86:C1:201:OHX:N1   | 2.66                     | 0.44              |
| 6:S4:179:LYS:O     | 6:S4:194:THR:O     | 2.35                     | 0.44              |
| 9:S7:164:TYR:H     | 9:S7:164:TYR:HD2   | 1.63                     | 0.44              |
| 13:C1:18:HIS:O     | 86:C1:201:OHX:N6   | 2.50                     | 0.44              |
| 21:C9:23:GLN:HG2   | 21:C9:55:TYR:CG    | 2.53                     | 0.44              |
| 21:C9:118:PRO:O    | 21:C9:119:LYS:HB2  | 2.17                     | 0.44              |
| 22:D0:96:PRO:O     | 22:D0:100:VAL:HG23 | 2.18                     | 0.44              |
| 25:D3:57:LEU:HD22  | 32:E0:4:VAL:HG12   | 1.99                     | 0.44              |
| 26:D4:126:ALA:O    | 26:D4:129:VAL:HG12 | 2.18                     | 0.44              |
| 34:SR:128:ASP:O    | 34:SR:130:THR:HG23 | 2.16                     | 0.44              |
| 34:SR:272:ASP:OD1  | 34:SR:273:ASP:N    | 2.51                     | 0.44              |
| 36:1:7:C:H5'       | 45:L8:193:LYS:HB3  | 1.99                     | 0.44              |
| 36:1:650:C:H2'     | 36:1:651:G:C8      | 2.52                     | 0.44              |
| 36:1:781:G:N7      | 86:1:3945:OHX:N5   | 2.65                     | 0.44              |
| 36:1:1029:G:H2'    | 36:1:1030:A:C8     | 2.52                     | 0.44              |
| 36:1:1422:G:H21    | 43:L6:5:LYS:HZ3    | 1.66                     | 0.44              |
| 36:1:1460:A:H2'    | 36:1:1461:A:C8     | 2.52                     | 0.44              |
| 36:1:1579:C:N4     | 36:1:1580:A:H62    | 2.16                     | 0.44              |
| 36:1:1940:G:N2     | 36:1:3362:A:C8     | 2.83                     | 0.44              |
| 86:1:4007:OHX:N6   | 86:1:4175:OHX:N2   | 2.66                     | 0.44              |
| 39:L2:104:LEU:O    | 39:L2:139:HIS:HE1  | 2.01                     | 0.44              |
| 40:L3:286:GLY:HA3  | 40:L3:321:PHE:CZ   | 2.52                     | 0.44              |
| 40:L3:306:THR:OG1  | 40:L3:316:GLU:O    | 2.22                     | 0.44              |
| 41:L4:135:VAL:O    | 41:L4:140:HIS:HB2  | 2.17                     | 0.44              |
| 45:L8:116:VAL:HG21 | 45:L8:123:GLN:HA   | 1.99                     | 0.44              |
| 47:M0:74:LYS:HE3   | 47:M0:74:LYS:HB2   | 1.81                     | 0.44              |
| 48:M1:107:ASP:HA   | 48:M1:124:GLY:HA2  | 1.99                     | 0.44              |
| 49:M3:166:ALA:HB1  | 64:N8:147:LEU:HD21 | 2.00                     | 0.44              |
| 59:N3:81:GLN:O     | 59:N3:82:ALA:CB    | 2.65                     | 0.44              |
| 66:O0:17:VAL:CG2   | 66:O0:100:ILE:HG12 | 2.48                     | 0.44              |
| 79:Q3:45:LYS:HB2   | 79:Q3:45:LYS:HE3   | 1.57                     | 0.44              |
| 1:6:348:U:O4       | 86:6:2163:OHX:N4   | 2.51                     | 0.44              |
| 1:6:563:U:H4'      | 80:e0:17:GLN:OE1   | 2.18                     | 0.44              |
| 1:6:922:G:H2'      | 1:6:923:A:H8       | 1.83                     | 0.44              |
| 6:s4:118:GLU:HA    | 6:s4:121:TYR:CE1   | 2.52                     | 0.44              |
| 7:s5:164:PRO:HA    | 7:s5:167:ARG:HG3   | 2.00                     | 0.44              |
| 9:s7:44:LYS:NZ     | 9:s7:95:GLU:OE2    | 2.45                     | 0.44              |
| 13:c1:54:ILE:HD13  | 13:c1:54:ILE:HA    | 1.66                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:d0:34:LEU:HD21  | 22:d0:89:ARG:HD2   | 1.98                     | 0.44              |
| 35:sM:46:LYS:HA    | 36:5:1018:G:H4'    | 2.00                     | 0.44              |
| 36:5:408:A:N6      | 38:8:15:G:H1'      | 2.32                     | 0.44              |
| 36:5:837:A:H1'     | 79:q3:10:ILE:HD12  | 1.99                     | 0.44              |
| 36:5:1329:U:O5'    | 36:5:1329:U:H6     | 2.01                     | 0.44              |
| 36:5:1348:U:C5     | 36:5:1355:A:C5     | 3.06                     | 0.44              |
| 36:5:2656:A:H4'    | 36:5:2657:A:OP1    | 2.17                     | 0.44              |
| 36:5:2967:A:H5''   | 39:l2:213:GLY:CA   | 2.48                     | 0.44              |
| 39:l2:245:LEU:HA   | 39:l2:245:LEU:HD12 | 1.75                     | 0.44              |
| 41:l4:49:ALA:HA    | 41:l4:109:TRP:CZ2  | 2.52                     | 0.44              |
| 42:l5:155:THR:HB   | 42:l5:179:ARG:HA   | 2.00                     | 0.44              |
| 42:l5:257:GLU:H    | 42:l5:257:GLU:CD   | 2.26                     | 0.44              |
| 42:l5:271:LYS:HA   | 42:l5:271:LYS:HD3  | 1.86                     | 0.44              |
| 47:m0:29:SER:HA    | 47:m0:125:LEU:HD12 | 2.00                     | 0.44              |
| 49:m3:46:ILE:HD12  | 49:m3:49:ARG:NH1   | 2.33                     | 0.44              |
| 56:n0:169:SER:OG   | 56:n0:171:PHE:HB3  | 2.17                     | 0.44              |
| 59:n3:125:LEU:HB3  | 59:n3:126:TRP:CD1  | 2.53                     | 0.44              |
| 63:n7:15:ARG:NH2   | 70:o4:83:ASN:OD1   | 2.50                     | 0.44              |
| 64:n8:75:LEU:O     | 64:n8:77:LYS:N     | 2.50                     | 0.44              |
| 68:o2:24:ARG:HD3   | 68:o2:25:TYR:OH    | 2.17                     | 0.44              |
| 69:o3:44:TYR:HA    | 69:o3:47:LYS:HG3   | 1.98                     | 0.44              |
| 79:q3:49:ARG:HD3   | 79:q3:51:ALA:C     | 2.42                     | 0.44              |
| 1:2:755:A:H2'      | 1:2:756:A:H8       | 1.83                     | 0.44              |
| 1:2:902:G:O5'      | 1:2:902:G:H8       | 2.01                     | 0.44              |
| 1:2:1433:G:H2'     | 1:2:1434:U:C6      | 2.52                     | 0.44              |
| 86:2:2096:OHX:N3   | 86:2:2109:OHX:N5   | 2.66                     | 0.44              |
| 6:S4:71:LYS:CB     | 6:S4:76:VAL:HA     | 2.48                     | 0.44              |
| 10:S8:152:ILE:HD13 | 10:S8:157:GLU:OE1  | 2.17                     | 0.44              |
| 11:S9:109:LEU:HD13 | 11:S9:129:ILE:HD13 | 1.99                     | 0.44              |
| 13:C1:3:THR:HG1    | 13:C1:82:ARG:NE    | 2.16                     | 0.44              |
| 13:C1:57:LYS:HB2   | 13:C1:110:HIS:NE2  | 2.33                     | 0.44              |
| 14:C2:78:LEU:HD23  | 14:C2:78:LEU:HA    | 1.88                     | 0.44              |
| 15:C3:76:LYS:HB3   | 15:C3:76:LYS:HE3   | 1.75                     | 0.44              |
| 36:1:343:U:H1'     | 41:L4:95:ARG:HG3   | 1.98                     | 0.44              |
| 36:1:383:G:O6      | 86:1:4065:OHX:N2   | 2.51                     | 0.44              |
| 36:1:945:C:H2'     | 36:1:946:U:C6      | 2.53                     | 0.44              |
| 36:1:1818:U:H3'    | 36:1:1819:U:H5''   | 2.00                     | 0.44              |
| 36:1:2882:U:H2'    | 36:1:2883:U:C6     | 2.53                     | 0.44              |
| 37:3:20:A:C4       | 37:3:60:G:N2       | 2.85                     | 0.44              |
| 39:L2:183:GLY:O    | 39:L2:186:PHE:HB3  | 2.18                     | 0.44              |
| 42:L5:286:VAL:O    | 42:L5:290:ILE:HG12 | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:M1:28:ASP:HA    | 48:M1:31:THR:HG23  | 2.00                     | 0.44              |
| 54:M8:57:ILE:HG21  | 54:M8:57:ILE:HD13  | 1.69                     | 0.44              |
| 55:M9:81:ARG:HG3   | 55:M9:88:ARG:CZ    | 2.48                     | 0.44              |
| 68:O2:89:THR:HG22  | 68:O2:117:ILE:HG12 | 2.00                     | 0.44              |
| 70:O4:8:ARG:HH11   | 70:O4:8:ARG:CG     | 2.30                     | 0.44              |
| 73:O7:33:THR:HA    | 73:O7:39:TYR:O     | 2.18                     | 0.44              |
| 1:6:189:C:C2'      | 1:6:190:C:H5'      | 2.48                     | 0.44              |
| 1:6:830:U:C2'      | 1:6:831:U:H5'      | 2.47                     | 0.44              |
| 1:6:833:U:OP2      | 86:6:2202:OHX:N5   | 2.50                     | 0.44              |
| 1:6:1227:A:H3'     | 14:c2:118:ALA:HA   | 1.99                     | 0.44              |
| 1:6:1408:G:H2'     | 1:6:1409:G:O4'     | 2.18                     | 0.44              |
| 1:6:1699:G:N1      | 1:6:1701:A:H5''    | 2.33                     | 0.44              |
| 2:s0:9:LEU:HD13    | 2:s0:10:THR:O      | 2.17                     | 0.44              |
| 2:s0:52:LYS:NZ     | 23:d1:82:VAL:O     | 2.37                     | 0.44              |
| 2:s0:177:LEU:O     | 2:s0:181:VAL:HG22  | 2.17                     | 0.44              |
| 7:s5:37:GLN:CG     | 18:c6:53:LEU:HD13  | 2.47                     | 0.44              |
| 8:s6:31:ARG:NH1    | 8:s6:34:GLN:HE22   | 2.12                     | 0.44              |
| 10:s8:137:LYS:O    | 10:s8:140:GLU:N    | 2.40                     | 0.44              |
| 10:s8:184:LEU:HB3  | 10:s8:189:LEU:HB2  | 1.99                     | 0.44              |
| 22:d0:20:ILE:O     | 22:d0:94:GLU:HA    | 2.17                     | 0.44              |
| 27:d5:58:ARG:HA    | 27:d5:103:ARG:HB2  | 1.99                     | 0.44              |
| 80:e0:56:MET:HE2   | 80:e0:56:MET:HB2   | 1.81                     | 0.44              |
| 36:5:700:C:OP1     | 49:m3:65:TYR:OH    | 2.28                     | 0.44              |
| 36:5:999:G:C6      | 36:5:1000:C:N4     | 2.85                     | 0.44              |
| 36:5:1049:C:H2'    | 36:5:1050:U:H6     | 1.81                     | 0.44              |
| 36:5:1313:G:O6     | 86:5:4161:OHX:N6   | 2.50                     | 0.44              |
| 36:5:1488:G:O2'    | 70:o4:10:ARG:O     | 2.31                     | 0.44              |
| 36:5:2308:C:O2     | 86:5:4238:OHX:N1   | 2.51                     | 0.44              |
| 36:5:2594:C:H6     | 36:5:2594:C:OP2    | 2.01                     | 0.44              |
| 36:5:2973:G:C2'    | 36:5:2974:U:H5'    | 2.48                     | 0.44              |
| 36:5:3000:A:H2'    | 36:5:3001:C:H6     | 1.82                     | 0.44              |
| 86:5:4000:OHX:N2   | 86:5:4190:OHX:N5   | 2.65                     | 0.44              |
| 40:l3:53:MET:HE2   | 40:l3:77:THR:HG22  | 2.00                     | 0.44              |
| 40:l3:340:LYS:HE3  | 40:l3:340:LYS:HB3  | 1.79                     | 0.44              |
| 43:l6:40:LEU:HD13  | 43:l6:84:VAL:HG11  | 2.00                     | 0.44              |
| 45:l8:122:LYS:C    | 45:l8:124:ASP:H    | 2.25                     | 0.44              |
| 49:m3:144:THR:HG21 | 71:o5:118:ILE:HG21 | 1.99                     | 0.44              |
| 51:m5:141:ALA:O    | 51:m5:145:ASP:HB2  | 2.17                     | 0.44              |
| 52:m6:108:ILE:HA   | 52:m6:109:PRO:HD2  | 1.63                     | 0.44              |
| 69:o3:58:GLU:HA    | 69:o3:62:SER:O     | 2.17                     | 0.44              |
| 71:o5:85:THR:O     | 71:o5:89:ARG:HB2   | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:o5:86:ARG:HG3   | 71:o5:90:ARG:CZ    | 2.47                     | 0.44              |
| 72:o6:74:LYS:HG3   | 72:o6:80:PHE:CD2   | 2.52                     | 0.44              |
| 74:o8:11:PHE:O     | 74:o8:15:THR:HG23  | 2.18                     | 0.44              |
| 1:2:82:U:H2'       | 1:2:83:G:O4'       | 2.18                     | 0.44              |
| 1:2:637:C:OP1      | 24:D2:32:LYS:HG3   | 2.17                     | 0.44              |
| 1:2:819:G:O6       | 1:2:853:G:C6       | 2.71                     | 0.44              |
| 1:2:871:G:O2'      | 29:D7:66:PRO:HB2   | 2.17                     | 0.44              |
| 1:2:1096:C:H2'     | 1:2:1096:C:O2      | 2.16                     | 0.44              |
| 2:S0:76:ILE:HB     | 2:S0:123:VAL:HG22  | 1.99                     | 0.44              |
| 8:S6:23:ARG:O      | 8:S6:26:VAL:HG23   | 2.17                     | 0.44              |
| 8:S6:158:ILE:HD12  | 8:S6:158:ILE:HA    | 1.63                     | 0.44              |
| 13:C1:109:VAL:CG2  | 13:C1:139:VAL:HG23 | 2.47                     | 0.44              |
| 21:C9:57:ARG:CG    | 21:C9:57:ARG:HH11  | 2.30                     | 0.44              |
| 26:D4:54:ALA:HB2   | 26:D4:79:VAL:HG22  | 2.00                     | 0.44              |
| 29:D7:29:ARG:HH11  | 29:D7:29:ARG:CG    | 2.25                     | 0.44              |
| 34:SR:26:SER:OG    | 34:SR:75:ALA:O     | 2.33                     | 0.44              |
| 36:1:600:G:N7      | 86:1:4100:OHX:N1   | 2.65                     | 0.44              |
| 36:1:606:C:O2'     | 36:1:607:A:N3      | 2.50                     | 0.44              |
| 36:1:806:A:C4      | 36:1:936:A:C2      | 3.06                     | 0.44              |
| 36:1:3385:U:H2'    | 36:1:3386:G:O4'    | 2.18                     | 0.44              |
| 86:1:3964:OHX:N2   | 86:1:4143:OHX:N4   | 2.66                     | 0.44              |
| 86:1:4059:OHX:N4   | 86:1:4166:OHX:N3   | 2.65                     | 0.44              |
| 41:L4:156:LEU:HD22 | 41:L4:215:ILE:HD13 | 1.99                     | 0.44              |
| 44:L7:73:GLY:O     | 57:N1:143:THR:HB   | 2.18                     | 0.44              |
| 45:L8:136:LEU:HD11 | 45:L8:162:LEU:O    | 2.18                     | 0.44              |
| 51:M5:183:THR:O    | 51:M5:183:THR:HG23 | 2.18                     | 0.44              |
| 56:N0:131:LYS:HB2  | 56:N0:134:ASP:OD2  | 2.18                     | 0.44              |
| 57:N1:42:ILE:HG12  | 57:N1:96:ILE:HD11  | 2.00                     | 0.44              |
| 59:N3:86:ARG:HA    | 59:N3:91:VAL:O     | 2.18                     | 0.44              |
| 1:6:72:A:H5'       | 1:6:73:U:OP2       | 2.17                     | 0.44              |
| 1:6:93:A:H4'       | 1:6:94:U:OP2       | 2.18                     | 0.44              |
| 1:6:271:A:H5'      | 1:6:272:U:OP2      | 2.17                     | 0.44              |
| 1:6:532:U:H2'      | 1:6:533:U:O4'      | 2.17                     | 0.44              |
| 1:6:964:U:H4'      | 1:6:965:U:O4'      | 2.18                     | 0.44              |
| 1:6:1616:G:H4'     | 30:d8:18:ARG:NH1   | 2.33                     | 0.44              |
| 4:s2:49:LYS:HA     | 4:s2:49:LYS:HD3    | 1.71                     | 0.44              |
| 15:c3:54:LEU:HB3   | 15:c3:60:VAL:CG1   | 2.48                     | 0.44              |
| 17:c5:85:ILE:HG22  | 17:c5:112:LEU:HD23 | 2.00                     | 0.44              |
| 19:c7:34:LEU:HD22  | 19:c7:38:ILE:CD1   | 2.48                     | 0.44              |
| 19:c7:77:GLU:HG2   | 19:c7:80:ARG:HH21  | 1.82                     | 0.44              |
| 21:c9:16:ASN:HA    | 21:c9:56:LYS:HZ3   | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:d0:21:LYS:HA    | 22:d0:94:GLU:HG2   | 1.99                     | 0.44              |
| 23:d1:3:ASN:OD1    | 23:d1:7:GLN:HB2    | 2.17                     | 0.44              |
| 34:sR:129:LYS:HG2  | 34:sR:149:ASP:C    | 2.43                     | 0.44              |
| 36:5:507:U:H2'     | 36:5:508:U:C6      | 2.53                     | 0.44              |
| 36:5:2167:A:H2'    | 36:5:2168:A:C8     | 2.53                     | 0.44              |
| 36:5:2406:C:H2'    | 36:5:2407:C:C6     | 2.53                     | 0.44              |
| 36:5:2584:G:H3'    | 36:5:2585:G:H4'    | 1.99                     | 0.44              |
| 36:5:2896:A:H5''   | 36:5:2896:A:C8     | 2.52                     | 0.44              |
| 86:5:4187:OHX:N5   | 86:5:4189:OHX:N2   | 2.65                     | 0.44              |
| 41:l4:142:VAL:HB   | 41:l4:145:ILE:HD13 | 2.00                     | 0.44              |
| 42:l5:135:VAL:HG12 | 42:l5:136:GLU:H    | 1.82                     | 0.44              |
| 58:n2:59:ASP:OD1   | 58:n2:60:GLY:N     | 2.51                     | 0.44              |
| 59:n3:120:LYS:H    | 59:n3:137:VAL:HG23 | 1.83                     | 0.44              |
| 63:n7:97:SER:HB3   | 63:n7:99:GLU:HG2   | 1.98                     | 0.44              |
| 68:o2:71:HIS:CE1   | 68:o2:118:LYS:HD3  | 2.52                     | 0.44              |
| 70:o4:41:ARG:HG2   | 70:o4:56:THR:HG21  | 2.00                     | 0.44              |
| 83:p1:34:UNK:C     | 83:p1:36:UNK:N     | 2.81                     | 0.44              |
| 1:2:373:G:N7       | 86:2:2160:OHX:N6   | 2.66                     | 0.44              |
| 1:2:446:A:N6       | 1:2:461:G:H21      | 2.16                     | 0.44              |
| 1:2:705:U:H2'      | 1:2:706:A:C8       | 2.52                     | 0.44              |
| 1:2:1080:U:OP2     | 1:2:1080:U:H6      | 2.01                     | 0.44              |
| 1:2:1445:G:C4      | 33:E1:91:ILE:HB    | 2.53                     | 0.44              |
| 2:S0:122:ILE:HA    | 2:S0:144:ILE:O     | 2.18                     | 0.44              |
| 9:S7:39:ARG:N      | 9:S7:40:PRO:HD2    | 2.33                     | 0.44              |
| 9:S7:71:HIS:CG     | 9:S7:131:PHE:CZ    | 3.06                     | 0.44              |
| 15:C3:118:ILE:O    | 15:C3:122:ILE:HG13 | 2.17                     | 0.44              |
| 17:C5:126:VAL:HG13 | 17:C5:127:ARG:N    | 2.21                     | 0.44              |
| 22:D0:39:SER:HA    | 22:D0:42:VAL:HG12  | 1.99                     | 0.44              |
| 30:D8:12:VAL:HA    | 30:D8:30:VAL:HG12  | 1.98                     | 0.44              |
| 34:SR:228:LYS:HB2  | 34:SR:228:LYS:HE3  | 1.79                     | 0.44              |
| 36:1:96:G:P        | 64:N8:34:MET:HB2   | 2.58                     | 0.44              |
| 36:1:595:G:C8      | 36:1:609:G:C6      | 3.05                     | 0.44              |
| 36:1:2115:G:H22    | 36:1:2120:A:H1'    | 1.82                     | 0.44              |
| 36:1:2197:C:N4     | 36:1:2241:U:H2'    | 2.33                     | 0.44              |
| 36:1:3136:G:OP2    | 86:1:4103:OHX:N6   | 2.50                     | 0.44              |
| 36:1:3275:U:C5'    | 69:O3:68:TRP:HZ2   | 2.30                     | 0.44              |
| 40:L3:299:ASP:O    | 40:L3:300:ARG:HB2  | 2.17                     | 0.44              |
| 46:L9:26:LYS:HA    | 46:L9:35:THR:HG22  | 2.00                     | 0.44              |
| 48:M1:89:TYR:HB3   | 48:M1:169:ALA:CB   | 2.47                     | 0.44              |
| 49:M3:54:LEU:HG    | 49:M3:119:TYR:CD1  | 2.52                     | 0.44              |
| 49:M3:188:ARG:NH1  | 49:M3:192:GLU:OE1  | 2.50                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:M5:73:ARG:O    | 51:M5:74:PRO:O     | 2.36                     | 0.44              |
| 51:M5:194:GLN:HG2 | 51:M5:194:GLN:H    | 1.58                     | 0.44              |
| 52:M6:38:ALA:O    | 52:M6:41:LEU:HB2   | 2.18                     | 0.44              |
| 52:M6:46:GLU:OE2  | 52:M6:134:LYS:HE3  | 2.17                     | 0.44              |
| 56:N0:40:ARG:HA   | 56:N0:40:ARG:HD2   | 1.74                     | 0.44              |
| 56:N0:109:ASP:OD1 | 56:N0:113:ARG:NH1  | 2.50                     | 0.44              |
| 59:N3:120:LYS:N   | 59:N3:137:VAL:HG23 | 2.33                     | 0.44              |
| 63:N7:3:LYS:O     | 63:N7:5:LEU:N      | 2.51                     | 0.44              |
| 65:N9:28:LYS:HA   | 65:N9:28:LYS:HD3   | 1.57                     | 0.44              |
| 67:O1:51:LEU:HD22 | 67:O1:55:LEU:HD12  | 1.99                     | 0.44              |
| 76:Q0:85:LEU:HD23 | 76:Q0:85:LEU:HA    | 1.88                     | 0.44              |
| 1:6:1511:U:H2'    | 1:6:1512:G:C8      | 2.52                     | 0.44              |
| 86:6:2150:OHX:N3  | 86:c1:202:OHX:N6   | 2.66                     | 0.44              |
| 2:s0:147:THR:O    | 2:s0:161:PRO:HA    | 2.18                     | 0.44              |
| 4:s2:175:GLY:HA3  | 11:s9:53:ARG:NH2   | 2.33                     | 0.44              |
| 6:s4:102:VAL:HG23 | 6:s4:182:TYR:OH    | 2.18                     | 0.44              |
| 9:s7:155:ASP:OD2  | 9:s7:156:SER:N     | 2.47                     | 0.44              |
| 11:s9:129:ILE:HA  | 11:s9:134:ILE:HG12 | 1.98                     | 0.44              |
| 13:c1:131:ILE:HB  | 13:c1:135:VAL:HG12 | 2.00                     | 0.44              |
| 19:c7:33:ARG:HD2  | 34:sR:109:ASP:OD2  | 2.17                     | 0.44              |
| 23:d1:69:LEU:HA   | 23:d1:69:LEU:HD23  | 1.55                     | 0.44              |
| 34:sR:84:SER:OG   | 34:sR:85:TRP:N     | 2.50                     | 0.44              |
| 36:5:1232:C:H2'   | 36:5:1233:G:C8     | 2.52                     | 0.44              |
| 36:5:1407:A:H5'   | 68:o2:32:TRP:HB3   | 1.99                     | 0.44              |
| 36:5:1493:G:N7    | 75:o9:5:LYS:NZ     | 2.64                     | 0.44              |
| 36:5:2309:A:H4'   | 86:5:4196:OHX:N4   | 2.33                     | 0.44              |
| 36:5:2617:U:O3'   | 47:m0:116:ARG:NH2  | 2.47                     | 0.44              |
| 86:5:4000:OHX:N6  | 86:5:4190:OHX:N5   | 2.66                     | 0.44              |
| 86:5:4187:OHX:N5  | 86:5:4189:OHX:N6   | 2.66                     | 0.44              |
| 38:8:23:U:OP1     | 62:n6:16:ARG:NH2   | 2.48                     | 0.44              |
| 39:l2:56:ALA:HB2  | 39:l2:130:SER:CB   | 2.46                     | 0.44              |
| 48:m1:29:ARG:HE   | 48:m1:29:ARG:HB2   | 1.68                     | 0.44              |
| 48:m1:108:GLU:HA  | 48:m1:122:ILE:HG23 | 2.00                     | 0.44              |
| 54:m8:166:LEU:O   | 54:m8:167:SER:CB   | 2.64                     | 0.44              |
| 59:n3:33:ASN:HD22 | 59:n3:63:LYS:HB2   | 1.82                     | 0.44              |
| 72:o6:98:ARG:HB3  | 72:o6:99:ARG:H     | 1.56                     | 0.44              |
| 79:q3:50:GLY:O    | 79:q3:51:ALA:HB3   | 2.18                     | 0.44              |
| 1:2:245:U:O4      | 86:2:2094:OHX:N5   | 2.51                     | 0.43              |
| 1:2:733:A:H4'     | 1:2:734:A:C5       | 2.53                     | 0.43              |
| 1:2:943:C:H42     | 28:D6:15:ARG:HG2   | 1.83                     | 0.43              |
| 1:2:1555:A:OP2    | 17:C5:47:ARG:NH2   | 2.51                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 86:2:2116:OHX:N6  | 86:C1:201:OHX:N4  | 2.66                     | 0.43              |
| 9:S7:83:LYS:C     | 9:S7:85:PHE:H     | 2.26                     | 0.43              |
| 18:C6:54:LEU:HD22 | 18:C6:54:LEU:HA   | 1.85                     | 0.43              |
| 20:C8:11:PHE:HD2  | 20:C8:59:GLY:HA3  | 1.80                     | 0.43              |
| 25:D3:63:GLN:HA   | 25:D3:65:ASN:N    | 2.33                     | 0.43              |
| 27:D5:41:ILE:O    | 27:D5:75:LEU:HD13 | 2.18                     | 0.43              |
| 29:D7:3:LEU:HD23  | 29:D7:3:LEU:HA    | 1.66                     | 0.43              |
| 33:E1:108:VAL:HA  | 33:E1:113:LYS:O   | 2.18                     | 0.43              |
| 36:1:22:G:H1'     | 38:4:104:A:N3     | 2.33                     | 0.43              |
| 36:1:674:G:O4'    | 41:L4:117:GLU:HG3 | 2.18                     | 0.43              |
| 36:1:1607:U:O2'   | 36:1:1608:C:H5'   | 2.18                     | 0.43              |
| 36:1:1876:U:H5''  | 36:1:1876:U:H6    | 1.82                     | 0.43              |
| 37:3:5:G:OP1      | 48:M1:143:ARG:NH2 | 2.42                     | 0.43              |
| 38:4:141:C:H5'    | 51:M5:109:ARG:HD2 | 2.00                     | 0.43              |
| 41:L4:170:LYS:HG3 | 41:L4:175:HIS:HB2 | 2.00                     | 0.43              |
| 41:L4:180:LYS:HB3 | 41:L4:180:LYS:HE3 | 1.71                     | 0.43              |
| 42:L5:108:ARG:CZ  | 42:L5:253:PHE:HB2 | 2.47                     | 0.43              |
| 59:N3:33:ASN:ND2  | 59:N3:64:LYS:HD3  | 2.33                     | 0.43              |
| 63:N7:88:ASP:O    | 63:N7:121:ARG:NH2 | 2.51                     | 0.43              |
| 72:O6:97:SER:OG   | 72:O6:98:ARG:N    | 2.49                     | 0.43              |
| 73:O7:84:SER:O    | 73:O7:85:LYS:HB2  | 2.18                     | 0.43              |
| 76:Q0:78:ILE:HG12 | 76:Q0:83:LYS:HD2  | 2.00                     | 0.43              |
| 78:Q2:83:LEU:HD23 | 78:Q2:83:LEU:HA   | 1.80                     | 0.43              |
| 1:6:675:U:H2'     | 1:6:676:G:C8      | 2.53                     | 0.43              |
| 1:6:1636:C:C2     | 1:6:1765:A:N6     | 2.86                     | 0.43              |
| 2:s0:6:THR:OG1    | 2:s0:191:ARG:HD3  | 2.18                     | 0.43              |
| 2:s0:190:ASP:C    | 2:s0:192:THR:H    | 2.26                     | 0.43              |
| 3:s1:67:GLU:CD    | 3:s1:83:LYS:HE2   | 2.43                     | 0.43              |
| 9:s7:115:SER:O    | 9:s7:115:SER:OG   | 2.29                     | 0.43              |
| 20:c8:35:ILE:HB   | 20:c8:38:VAL:CG2  | 2.47                     | 0.43              |
| 20:c8:108:LYS:HD3 | 20:c8:108:LYS:HA  | 1.79                     | 0.43              |
| 22:d0:83:GLU:OE1  | 22:d0:85:ARG:NE   | 2.48                     | 0.43              |
| 27:d5:60:VAL:HG13 | 27:d5:101:TYR:HB2 | 2.00                     | 0.43              |
| 36:5:29:C:O3'     | 51:m5:172:ARG:NH1 | 2.51                     | 0.43              |
| 36:5:784:A:C6     | 54:m8:93:ILE:HG23 | 2.53                     | 0.43              |
| 36:5:1255:C:H2'   | 36:5:1256:G:H8    | 1.83                     | 0.43              |
| 36:5:1573:G:C5    | 36:5:1574:C:H1'   | 2.53                     | 0.43              |
| 36:5:1811:G:H2'   | 36:5:1812:G:O4'   | 2.18                     | 0.43              |
| 36:5:2409:G:H4'   | 36:5:2410:U:OP2   | 2.18                     | 0.43              |
| 36:5:2875:U:H2'   | 36:5:2876:C:O5'   | 2.17                     | 0.43              |
| 36:5:3139:A:H4'   | 40:l3:20:LYS:HD3  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:3272:C:O2     | 43:l6:80:ASN:HB2   | 2.18                     | 0.43              |
| 86:5:4011:OHX:N4   | 86:5:4198:OHX:N2   | 2.66                     | 0.43              |
| 41:l4:324:LEU:O    | 41:l4:327:LEU:O    | 2.36                     | 0.43              |
| 41:l4:338:LYS:HD3  | 41:l4:338:LYS:HA   | 1.53                     | 0.43              |
| 48:m1:10:ARG:HB3   | 48:m1:152:HIS:CE1  | 2.53                     | 0.43              |
| 48:m1:21:ILE:HG12  | 48:m1:125:MET:HB3  | 1.98                     | 0.43              |
| 55:m9:4:LEU:HD22   | 55:m9:7:GLN:HG3    | 1.98                     | 0.43              |
| 56:n0:82:ASP:OD1   | 56:n0:87:THR:HB    | 2.17                     | 0.43              |
| 61:n5:108:LEU:HD23 | 61:n5:108:LEU:HA   | 1.71                     | 0.43              |
| 64:n8:126:LYS:HA   | 64:n8:146:GLU:O    | 2.17                     | 0.43              |
| 1:2:65:A:OP1       | 8:S6:176:GLN:NE2   | 2.42                     | 0.43              |
| 1:2:625:C:H2'      | 1:2:626:U:C6       | 2.53                     | 0.43              |
| 1:2:647:G:N2       | 1:2:687:G:H22      | 2.16                     | 0.43              |
| 1:2:1274:C:H41     | 35:SM:95:SER:HA    | 1.83                     | 0.43              |
| 1:2:1637:C:O2'     | 35:SM:94:HIS:HE1   | 2.01                     | 0.43              |
| 1:2:1681:A:H1'     | 8:S6:66:GLY:HA2    | 1.99                     | 0.43              |
| 14:C2:60:VAL:HG22  | 14:C2:122:VAL:HG22 | 1.99                     | 0.43              |
| 22:D0:43:LYS:HA    | 22:D0:43:LYS:HD2   | 1.65                     | 0.43              |
| 35:SM:84:LYS:HG2   | 35:SM:86:ASN:N     | 2.33                     | 0.43              |
| 36:1:279:U:H2'     | 36:1:280:U:C6      | 2.53                     | 0.43              |
| 36:1:815:G:C6      | 36:1:906:A:C4      | 3.06                     | 0.43              |
| 36:1:860:G:OP1     | 79:Q3:17:ARG:NH1   | 2.51                     | 0.43              |
| 36:1:1370:G:H5''   | 64:N8:18:GLY:O     | 2.18                     | 0.43              |
| 36:1:1546:A:N7     | 51:M5:71:ARG:NH1   | 2.66                     | 0.43              |
| 36:1:2263:C:OP1    | 86:1:3990:OHX:N1   | 2.51                     | 0.43              |
| 36:1:2402:A:C2     | 36:1:2871:G:C6     | 3.06                     | 0.43              |
| 36:1:2574:G:H2'    | 36:1:2575:G:H8     | 1.82                     | 0.43              |
| 36:1:3364:C:H2'    | 36:1:3365:U:C6     | 2.53                     | 0.43              |
| 86:1:4135:OHX:N5   | 86:1:4167:OHX:N6   | 2.66                     | 0.43              |
| 40:L3:4:ARG:O      | 40:L3:5:LYS:HB2    | 2.18                     | 0.43              |
| 40:L3:84:VAL:HG13  | 40:L3:162:VAL:HB   | 2.00                     | 0.43              |
| 40:L3:320:ASP:OD2  | 40:L3:320:ASP:N    | 2.50                     | 0.43              |
| 42:L5:120:LYS:O    | 42:L5:248:ARG:NH2  | 2.50                     | 0.43              |
| 47:M0:48:LEU:O     | 47:M0:139:ARG:HA   | 2.17                     | 0.43              |
| 51:M5:93:LYS:O     | 51:M5:94:TYR:HB3   | 2.18                     | 0.43              |
| 54:M8:150:VAL:HA   | 54:M8:153:PHE:CD1  | 2.52                     | 0.43              |
| 54:M8:161:LYS:O    | 54:M8:162:ALA:CB   | 2.64                     | 0.43              |
| 57:N1:105:PHE:O    | 57:N1:109:VAL:HG23 | 2.18                     | 0.43              |
| 61:N5:115:ARG:HD3  | 61:N5:121:LYS:HE2  | 2.00                     | 0.43              |
| 72:O6:45:ARG:NH2   | 72:O6:54:GLU:OE1   | 2.52                     | 0.43              |
| 1:6:488:G:H21      | 1:6:499:U:H3       | 1.65                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:1014:G:H2'     | 1:6:1015:U:O4'     | 2.19                     | 0.43              |
| 1:6:1333:C:C4'     | 5:s3:162:GLN:HG3   | 2.48                     | 0.43              |
| 1:6:1380:U:O2'     | 1:6:1516:A:N1      | 2.47                     | 0.43              |
| 1:6:1465:C:OP1     | 18:c6:139:GLN:NE2  | 2.52                     | 0.43              |
| 1:6:1504:G:H2'     | 1:6:1505:A:C8      | 2.53                     | 0.43              |
| 1:6:1620:C:H2'     | 1:6:1621:U:C6      | 2.53                     | 0.43              |
| 2:s0:90:ALA:HA     | 2:s0:95:ALA:HB3    | 2.00                     | 0.43              |
| 4:s2:41:LEU:HD13   | 4:s2:68:ILE:HD13   | 2.01                     | 0.43              |
| 4:s2:229:LEU:HD23  | 23:d1:23:ILE:HD11  | 1.99                     | 0.43              |
| 6:s4:95:THR:CG2    | 6:s4:97:GLU:HG2    | 2.48                     | 0.43              |
| 7:s5:175:LEU:HD23  | 7:s5:197:GLU:HG3   | 2.01                     | 0.43              |
| 11:s9:101:VAL:HG23 | 11:s9:102:GLU:OE2  | 2.18                     | 0.43              |
| 11:s9:108:ARG:HB2  | 11:s9:111:THR:HG23 | 1.99                     | 0.43              |
| 12:c0:21:VAL:HG12  | 12:c0:66:TYR:HD2   | 1.83                     | 0.43              |
| 19:c7:13:SER:CB    | 19:c7:54:THR:HG22  | 2.47                     | 0.43              |
| 19:c7:47:ARG:NH1   | 19:c7:48:ASN:OD1   | 2.51                     | 0.43              |
| 20:c8:139:LYS:O    | 20:c8:143:ARG:NH1  | 2.51                     | 0.43              |
| 21:c9:131:ASP:O    | 21:c9:135:ILE:HG23 | 2.18                     | 0.43              |
| 23:d1:43:GLY:O     | 23:d1:44:ARG:C     | 2.61                     | 0.43              |
| 28:d6:36:ILE:HD12  | 28:d6:36:ILE:N     | 2.33                     | 0.43              |
| 35:sM:57:ASN:O     | 35:sM:61:ILE:HG22  | 2.18                     | 0.43              |
| 36:5:1845:G:O2'    | 73:o7:8:PHE:HD2    | 2.02                     | 0.43              |
| 36:5:1932:A:H5'    | 36:5:1933:A:OP2    | 2.18                     | 0.43              |
| 36:5:2102:U:H2'    | 36:5:2103:U:C6     | 2.52                     | 0.43              |
| 36:5:2344:U:H2'    | 36:5:2345:A:C8     | 2.53                     | 0.43              |
| 36:5:2542:U:H1'    | 36:5:2543:U:C5     | 2.52                     | 0.43              |
| 36:5:2581:U:H2'    | 36:5:2582:C:C6     | 2.53                     | 0.43              |
| 36:5:3167:A:H2'    | 36:5:3168:A:O4'    | 2.17                     | 0.43              |
| 40:l3:2:SER:O      | 40:l3:3:HIS:CB     | 2.66                     | 0.43              |
| 40:l3:137:TYR:O    | 40:l3:139:GLN:N    | 2.50                     | 0.43              |
| 41:l4:57:GLY:HA3   | 41:l4:98:ARG:N     | 2.33                     | 0.43              |
| 41:l4:361:HIS:O    | 56:n0:28:ARG:NH2   | 2.48                     | 0.43              |
| 42:l5:261:THR:OG1  | 42:l5:264:GLN:HG3  | 2.18                     | 0.43              |
| 54:m8:122:ILE:HG22 | 54:m8:123:THR:O    | 2.18                     | 0.43              |
| 61:n5:103:TYR:O    | 61:n5:105:VAL:HG23 | 2.18                     | 0.43              |
| 65:n9:54:LEU:HD23  | 65:n9:54:LEU:HA    | 1.75                     | 0.43              |
| 66:o0:10:ILE:HD12  | 66:o0:10:ILE:HA    | 1.86                     | 0.43              |
| 71:o5:30:GLU:O     | 71:o5:34:GLN:HG3   | 2.18                     | 0.43              |
| 72:o6:59:ASP:O     | 72:o6:63:ASN:HB2   | 2.18                     | 0.43              |
| 1:2:1166:A:H2'     | 1:2:1167:G:O4'     | 2.18                     | 0.43              |
| 1:2:1383:G:OP1     | 22:D0:87:HIS:ND1   | 2.42                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2:1571:C:OP2     | 86:2:2155:OHX:N1  | 2.51                     | 0.43              |
| 1:2:1734:U:O2'     | 1:2:1735:U:H5'    | 2.19                     | 0.43              |
| 2:S0:120:LEU:HD12  | 2:S0:142:PRO:O    | 2.18                     | 0.43              |
| 3:S1:23:PRO:O      | 3:S1:27:LYS:HG2   | 2.18                     | 0.43              |
| 3:S1:91:VAL:HG23   | 3:S1:96:LEU:HB3   | 2.00                     | 0.43              |
| 6:S4:222:LEU:HB3   | 6:S4:223:ASN:H    | 1.64                     | 0.43              |
| 10:S8:96:LEU:HD13  | 10:S8:179:CYS:SG  | 2.59                     | 0.43              |
| 18:C6:45:ARG:HG2   | 18:C6:49:TYR:CE2  | 2.53                     | 0.43              |
| 19:C7:71:PHE:CD1   | 19:C7:73:LEU:HB3  | 2.53                     | 0.43              |
| 21:C9:23:GLN:C     | 21:C9:25:GLN:H    | 2.26                     | 0.43              |
| 28:D6:73:TYR:CZ    | 28:D6:82:ARG:HD2  | 2.54                     | 0.43              |
| 33:E1:113:LYS:H    | 33:E1:113:LYS:HD2 | 1.82                     | 0.43              |
| 34:SR:248:ASN:OD1  | 34:SR:248:ASN:N   | 2.51                     | 0.43              |
| 35:SM:82:THR:HB    | 35:SM:83:LYS:H    | 1.40                     | 0.43              |
| 36:1:346:C:OP1     | 41:L4:52:VAL:HG22 | 2.18                     | 0.43              |
| 36:1:546:C:H5'     | 36:1:547:G:O4'    | 2.18                     | 0.43              |
| 36:1:553:U:H2'     | 36:1:554:A:O4'    | 2.17                     | 0.43              |
| 36:1:695:C:OP1     | 41:L4:271:LYS:NZ  | 2.48                     | 0.43              |
| 36:1:1276:U:OP1    | 86:1:4089:OHX:N4  | 2.52                     | 0.43              |
| 36:1:1486:G:O6     | 86:1:3980:OHX:N5  | 2.51                     | 0.43              |
| 36:1:1576:G:N7     | 36:1:1577:G:C6    | 2.87                     | 0.43              |
| 36:1:2402:A:OP2    | 86:1:4092:OHX:N6  | 2.51                     | 0.43              |
| 36:1:2606:G:H2'    | 36:1:2606:G:N3    | 2.33                     | 0.43              |
| 36:1:2612:U:H2'    | 36:1:2613:U:O4'   | 2.18                     | 0.43              |
| 36:1:3115:C:O2'    | 36:1:3117:C:N4    | 2.45                     | 0.43              |
| 41:L4:265:GLU:H    | 41:L4:265:GLU:CD  | 2.25                     | 0.43              |
| 41:L4:311:HIS:NE2  | 41:L4:314:LYS:HA  | 2.34                     | 0.43              |
| 47:M0:61:SER:HB2   | 47:M0:63:GLU:HG2  | 1.99                     | 0.43              |
| 47:M0:188:GLY:O    | 47:M0:190:VAL:N   | 2.51                     | 0.43              |
| 52:M6:16:VAL:HG23  | 52:M6:42:ASN:O    | 2.19                     | 0.43              |
| 57:N1:79:MET:HB3   | 57:N1:84:TYR:CE2  | 2.53                     | 0.43              |
| 76:Q0:127:LEU:HD13 | 76:Q0:128:LYS:HG2 | 2.00                     | 0.43              |
| 1:6:590:C:H5''     | 80:e0:43:ARG:HH12 | 1.83                     | 0.43              |
| 1:6:758:U:OP1      | 11:s9:7:THR:HG21  | 2.17                     | 0.43              |
| 1:6:1045:C:OP1     | 3:s1:153:HIS:HE1  | 2.01                     | 0.43              |
| 1:6:1124:A:O2'     | 1:6:1125:A:H5'    | 2.18                     | 0.43              |
| 1:6:1234:A:H4'     | 33:e1:146:SER:OG  | 2.19                     | 0.43              |
| 1:6:1441:C:H2'     | 1:6:1442:U:C6     | 2.52                     | 0.43              |
| 1:6:1621:U:C2      | 1:6:1622:G:C8     | 3.06                     | 0.43              |
| 2:s0:7:PHE:HZ      | 23:d1:43:GLY:HA2  | 1.83                     | 0.43              |
| 5:s3:224:ASP:OD1   | 34:sR:228:LYS:HD2 | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:s5:92:ARG:HH11   | 7:s5:92:ARG:CG    | 2.24                     | 0.43              |
| 8:s6:2:LYS:HB3     | 8:s6:108:VAL:HG13 | 2.00                     | 0.43              |
| 10:s8:10:LYS:HG2   | 13:c1:133:LYS:HE3 | 2.01                     | 0.43              |
| 16:c4:45:GLY:HA2   | 16:c4:54:GLU:HG2  | 1.99                     | 0.43              |
| 18:c6:115:THR:HG22 | 18:c6:116:LEU:N   | 2.32                     | 0.43              |
| 21:c9:5:SER:OG     | 21:c9:7:ARG:HG3   | 2.19                     | 0.43              |
| 28:d6:61:GLU:O     | 28:d6:62:TYR:HB3  | 2.18                     | 0.43              |
| 36:5:599:C:OP1     | 41:l4:332:LYS:HE3 | 2.18                     | 0.43              |
| 36:5:1098:A:C2'    | 36:5:1099:A:H5'   | 2.49                     | 0.43              |
| 36:5:1635:G:OP1    | 63:n7:107:ARG:NH2 | 2.46                     | 0.43              |
| 36:5:2093:A:H3'    | 36:5:2093:A:N3    | 2.34                     | 0.43              |
| 36:5:2973:G:H2'    | 36:5:2974:U:H5'   | 2.00                     | 0.43              |
| 36:5:3259:U:C5'    | 36:5:3259:U:H6    | 2.31                     | 0.43              |
| 36:5:3390:G:C2'    | 36:5:3391:A:H5'   | 2.49                     | 0.43              |
| 86:5:4093:OHX:N5   | 86:5:4199:OHX:N1  | 2.65                     | 0.43              |
| 37:7:23:A:C6       | 37:7:24:A:C6      | 3.07                     | 0.43              |
| 40:l3:128:LYS:HB3  | 40:l3:128:LYS:HE2 | 1.84                     | 0.43              |
| 41:l4:283:THR:HB   | 41:l4:285:ASP:H   | 1.83                     | 0.43              |
| 46:l9:13:PRO:HG2   | 46:l9:16:VAL:HG11 | 2.00                     | 0.43              |
| 81:m2:120:UNK:C    | 81:m2:122:UNK:N   | 2.82                     | 0.43              |
| 52:m6:167:TYR:CD1  | 52:m6:167:TYR:C   | 2.92                     | 0.43              |
| 57:n1:54:HIS:CE1   | 57:n1:55:LYS:HG2  | 2.54                     | 0.43              |
| 73:o7:22:CYS:SG    | 73:o7:24:ARG:HG3  | 2.59                     | 0.43              |
| 1:2:443:C:OP2      | 26:D4:105:ARG:HB3 | 2.18                     | 0.43              |
| 1:2:452:A:H3'      | 1:2:453:U:C5      | 2.54                     | 0.43              |
| 1:2:579:A:C2       | 5:S3:143:ARG:HG3  | 2.42                     | 0.43              |
| 1:2:887:A:C1'      | 16:C4:122:PRO:HB3 | 2.45                     | 0.43              |
| 1:2:1178:G:H2'     | 1:2:1179:G:O4'    | 2.19                     | 0.43              |
| 1:2:1515:A:OP2     | 5:S3:7:LYS:HB2    | 2.18                     | 0.43              |
| 1:2:1587:A:H2'     | 1:2:1588:G:H8     | 1.82                     | 0.43              |
| 2:S0:162:CYS:HB3   | 2:S0:163:ASN:H    | 1.51                     | 0.43              |
| 7:S5:33:VAL:O      | 7:S5:37:GLN:HB2   | 2.18                     | 0.43              |
| 18:C6:44:LEU:O     | 18:C6:47:LYS:HB2  | 2.17                     | 0.43              |
| 20:C8:18:LEU:HD13  | 20:C8:18:LEU:HA   | 1.82                     | 0.43              |
| 20:C8:142:GLY:O    | 20:C8:145:ARG:HD2 | 2.17                     | 0.43              |
| 27:D5:42:LEU:O     | 27:D5:44:GLN:N    | 2.51                     | 0.43              |
| 27:D5:82:HIS:O     | 27:D5:85:LYS:HB3  | 2.19                     | 0.43              |
| 28:D6:85:ARG:HD3   | 28:D6:85:ARG:HA   | 1.57                     | 0.43              |
| 29:D7:67:THR:HG22  | 29:D7:68:GLY:H    | 1.82                     | 0.43              |
| 36:1:564:G:H2'     | 36:1:565:U:C6     | 2.54                     | 0.43              |
| 36:1:1597:C:H2'    | 36:1:1598:G:C8    | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:2341:A:P      | 40:L3:247:ARG:HH22 | 2.42                     | 0.43              |
| 36:1:2367:A:H2'    | 36:1:2368:A:O4'    | 2.18                     | 0.43              |
| 36:1:2850:G:O6     | 86:1:4079:OHX:N6   | 2.51                     | 0.43              |
| 36:1:3274:A:H2'    | 53:M7:171:ARG:NH1  | 2.34                     | 0.43              |
| 86:1:4056:OHX:N5   | 86:1:4163:OHX:N1   | 2.67                     | 0.43              |
| 86:1:4088:OHX:N6   | 86:1:4157:OHX:N3   | 2.66                     | 0.43              |
| 40:L3:361:THR:HG23 | 40:L3:371:GLN:O    | 2.17                     | 0.43              |
| 41:L4:295:ILE:O    | 41:L4:299:ILE:HG12 | 2.19                     | 0.43              |
| 42:L5:22:ARG:NH2   | 42:L5:28:THR:OG1   | 2.50                     | 0.43              |
| 48:M1:25:GLU:OE2   | 48:M1:29:ARG:HD2   | 2.19                     | 0.43              |
| 52:M6:16:VAL:HG21  | 52:M6:43:ILE:HG12  | 1.99                     | 0.43              |
| 64:N8:65:GLN:O     | 64:N8:66:ALA:CB    | 2.65                     | 0.43              |
| 69:O3:38:PRO:HD2   | 69:O3:39:GLN:OE1   | 2.18                     | 0.43              |
| 78:Q2:65:THR:OG1   | 78:Q2:87:ARG:NH1   | 2.49                     | 0.43              |
| 1:6:859:A:C5       | 15:c3:73:ARG:HD3   | 2.53                     | 0.43              |
| 1:6:1270:G:O2'     | 33:e1:79:LYS:HB2   | 2.19                     | 0.43              |
| 1:6:1363:U:O2'     | 1:6:1364:G:H5'     | 2.18                     | 0.43              |
| 6:s4:126:VAL:CG2   | 6:s4:156:VAL:HA    | 2.48                     | 0.43              |
| 6:s4:191:ARG:CZ    | 6:s4:245:LYS:HD2   | 2.48                     | 0.43              |
| 18:c6:102:LYS:HB3  | 18:c6:102:LYS:HE2  | 1.74                     | 0.43              |
| 20:c8:28:ILE:HG13  | 20:c8:28:ILE:H     | 1.59                     | 0.43              |
| 25:d3:135:LEU:HD23 | 25:d3:135:LEU:HA   | 1.85                     | 0.43              |
| 34:sR:10:ARG:HD3   | 34:sR:10:ARG:HA    | 1.76                     | 0.43              |
| 36:5:65:A:C4       | 36:5:110:G:N7      | 2.86                     | 0.43              |
| 36:5:67:A:OP1      | 86:5:3955:OHX:N6   | 2.52                     | 0.43              |
| 36:5:1298:C:O3'    | 76:q0:113:ARG:NH1  | 2.51                     | 0.43              |
| 36:5:1394:A:H4'    | 36:5:1420:C:H4'    | 2.01                     | 0.43              |
| 36:5:1468:A:N1     | 36:5:1880:U:O2'    | 2.50                     | 0.43              |
| 36:5:1480:G:N2     | 36:5:1872:C:C5     | 2.86                     | 0.43              |
| 36:5:1483:G:C8     | 36:5:1485:G:C8     | 3.06                     | 0.43              |
| 36:5:1816:A:O2'    | 36:5:1817:G:OP1    | 2.32                     | 0.43              |
| 38:8:124:G:OP2     | 86:8:222:OHX:N2    | 2.52                     | 0.43              |
| 45:l8:123:GLN:O    | 45:l8:125:ALA:N    | 2.41                     | 0.43              |
| 46:l9:188:THR:HG22 | 46:l9:189:GLU:N    | 2.33                     | 0.43              |
| 48:m1:17:LEU:HD21  | 48:m1:19:LEU:HD21  | 2.00                     | 0.43              |
| 57:n1:31:LEU:HD23  | 57:n1:31:LEU:HA    | 1.77                     | 0.43              |
| 66:o0:30:THR:O     | 66:o0:34:LEU:N     | 2.46                     | 0.43              |
| 68:o2:64:LYS:HD3   | 68:o2:65:PHE:CE2   | 2.52                     | 0.43              |
| 70:o4:74:ARG:CD    | 70:o4:85:VAL:HG21  | 2.48                     | 0.43              |
| 71:o5:47:VAL:O     | 71:o5:51:ILE:HG13  | 2.19                     | 0.43              |
| 74:o8:19:ASP:OD2   | 74:o8:19:ASP:N     | 2.46                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2:66:U:O3'       | 8:S6:171:LYS:NZ   | 2.50                     | 0.43              |
| 1:2:1061:A:H2'     | 1:2:1062:A:H5'    | 2.00                     | 0.43              |
| 1:2:1168:U:H2'     | 1:2:1169:G:H5'    | 2.01                     | 0.43              |
| 1:2:1484:G:O4'     | 1:2:1607:G:H4'    | 2.19                     | 0.43              |
| 86:2:2161:OHX:N5   | 11:S9:8:TYR:O     | 2.52                     | 0.43              |
| 3:S1:131:ASP:O     | 3:S1:133:TYR:N    | 2.44                     | 0.43              |
| 8:S6:110:ALA:O     | 8:S6:111:LEU:HD23 | 2.18                     | 0.43              |
| 9:S7:122:HIS:HA    | 9:S7:125:ILE:HD12 | 2.01                     | 0.43              |
| 36:1:20:A:P        | 71:O5:90:ARG:NH1  | 2.92                     | 0.43              |
| 36:1:345:G:H2'     | 38:4:25:G:O2'     | 2.18                     | 0.43              |
| 36:1:1246:G:H8     | 36:1:1246:G:OP1   | 2.02                     | 0.43              |
| 36:1:1256:G:O6     | 36:1:1261:G:N2    | 2.50                     | 0.43              |
| 36:1:3186:A:O2'    | 46:L9:42:ASP:HA   | 2.18                     | 0.43              |
| 86:1:4088:OHX:N5   | 86:1:4157:OHX:N1  | 2.66                     | 0.43              |
| 41:L4:222:VAL:HA   | 41:L4:223:PRO:HD3 | 1.82                     | 0.43              |
| 42:L5:49:TYR:CD1   | 42:L5:66:SER:HB3  | 2.53                     | 0.43              |
| 42:L5:163:LEU:HD11 | 42:L5:175:HIS:CG  | 2.53                     | 0.43              |
| 54:M8:176:ARG:HA   | 54:M8:182:LYS:O   | 2.18                     | 0.43              |
| 61:N5:73:MET:HE1   | 61:N5:141:TYR:CE1 | 2.52                     | 0.43              |
| 64:N8:116:GLY:HA2  | 64:N8:137:LYS:HZ3 | 1.83                     | 0.43              |
| 78:Q2:63:LYS:HD2   | 78:Q2:87:ARG:NH2  | 2.33                     | 0.43              |
| 1:6:74:U:H3'       | 1:6:75:U:H3'      | 2.00                     | 0.43              |
| 1:6:119:A:H1'      | 1:6:397:A:C5      | 2.53                     | 0.43              |
| 1:6:862:A:H4'      | 1:6:863:A:O5'     | 2.19                     | 0.43              |
| 1:6:901:G:N1       | 1:6:902:G:C6      | 2.86                     | 0.43              |
| 3:s1:157:GLN:O     | 3:s1:160:HIS:HB2  | 2.18                     | 0.43              |
| 6:s4:57:ASN:HB2    | 6:s4:60:GLU:H     | 1.84                     | 0.43              |
| 28:d6:30:ILE:HG13  | 28:d6:31:PRO:HD2  | 1.99                     | 0.43              |
| 34:sR:159:ASN:OD1  | 34:sR:163:ASP:HA  | 2.19                     | 0.43              |
| 34:sR:267:PRO:HD2  | 34:sR:269:TYR:HE1 | 1.83                     | 0.43              |
| 36:5:208:C:H2'     | 36:5:209:A:O4'    | 2.19                     | 0.43              |
| 36:5:279:U:H2'     | 36:5:280:U:C6     | 2.53                     | 0.43              |
| 36:5:438:A:C8      | 36:5:439:C:C5     | 3.03                     | 0.43              |
| 36:5:1366:A:C2     | 36:5:1367:G:C4    | 3.06                     | 0.43              |
| 36:5:1525:G:C6     | 36:5:1526:U:O4    | 2.72                     | 0.43              |
| 36:5:1556:C:H2'    | 36:5:2169:G:H1    | 1.84                     | 0.43              |
| 36:5:2339:C:OP2    | 59:n3:48:ARG:HG3  | 2.19                     | 0.43              |
| 36:5:2865:U:OP1    | 47:m0:115:MET:HB2 | 2.18                     | 0.43              |
| 36:5:2953:U:H2'    | 36:5:2954:U:H2'   | 2.01                     | 0.43              |
| 36:5:3163:A:N6     | 36:5:3164:C:H42   | 2.17                     | 0.43              |
| 36:5:3194:C:H2'    | 36:5:3195:U:H3'   | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:l5:211:LEU:HD23 | 42:l5:211:LEU:HA   | 1.88                     | 0.43              |
| 46:l9:162:GLN:NE2  | 76:q0:89:TYR:CD1   | 2.86                     | 0.43              |
| 46:l9:171:ASP:OD2  | 46:l9:173:ARG:NH1  | 2.51                     | 0.43              |
| 51:m5:180:PHE:O    | 51:m5:184:LYS:HB2  | 2.18                     | 0.43              |
| 63:n7:64:LYS:HE2   | 63:n7:64:LYS:HB2   | 1.82                     | 0.43              |
| 68:o2:24:ARG:HG2   | 68:o2:25:TYR:CE2   | 2.54                     | 0.43              |
| 71:o5:105:ARG:O    | 71:o5:109:ILE:HG13 | 2.19                     | 0.43              |
| 1:2:459:G:O2'      | 1:2:460:A:OP1      | 2.32                     | 0.43              |
| 1:2:1192:C:H5'     | 18:C6:142:TYR:HA   | 2.01                     | 0.43              |
| 1:2:1410:A:H5''    | 18:C6:118:ILE:HD13 | 2.00                     | 0.43              |
| 3:S1:158:SER:O     | 3:S1:162:ARG:HG3   | 2.18                     | 0.43              |
| 3:S1:193:ILE:O     | 3:S1:197:ILE:HG12  | 2.19                     | 0.43              |
| 5:S3:162:GLN:OE1   | 5:S3:165:ASN:ND2   | 2.40                     | 0.43              |
| 5:S3:216:PRO:HB2   | 5:S3:217:ILE:H     | 1.56                     | 0.43              |
| 5:S3:224:ASP:OD1   | 34:SR:228:LYS:HD2  | 2.19                     | 0.43              |
| 8:S6:55:GLY:N      | 8:S6:63:MET:HE3    | 2.34                     | 0.43              |
| 10:S8:76:THR:HB    | 10:S8:105:ASP:HB2  | 2.01                     | 0.43              |
| 12:C0:32:HIS:NE2   | 12:C0:35:ILE:HG13  | 2.34                     | 0.43              |
| 17:C5:64:LYS:HA    | 17:C5:73:PRO:HB3   | 2.01                     | 0.43              |
| 18:C6:143:ARG:HE   | 18:C6:143:ARG:HB3  | 1.66                     | 0.43              |
| 21:C9:125:SER:OG   | 21:C9:128:GLY:N    | 2.52                     | 0.43              |
| 22:D0:77:LYS:H     | 22:D0:77:LYS:HG2   | 1.59                     | 0.43              |
| 29:D7:8:LEU:HD23   | 29:D7:8:LEU:HA     | 1.86                     | 0.43              |
| 32:E0:14:VAL:O     | 32:E0:18:THR:HG23  | 2.18                     | 0.43              |
| 33:E1:103:LEU:HD23 | 33:E1:103:LEU:HA   | 1.69                     | 0.43              |
| 34:SR:245:PHE:O    | 34:SR:294:TRP:CD1  | 2.72                     | 0.43              |
| 36:1:608:A:C4      | 43:L6:22:ARG:NH1   | 2.87                     | 0.43              |
| 36:1:1390:A:N3     | 36:1:1390:A:H5'    | 2.33                     | 0.43              |
| 36:1:2184:U:OP1    | 39:L2:209:HIS:HE1  | 2.01                     | 0.43              |
| 36:1:2260:U:H2'    | 36:1:2261:G:O4'    | 2.19                     | 0.43              |
| 36:1:2854:U:P      | 47:M0:3:ARG:HH22   | 2.40                     | 0.43              |
| 86:1:3980:OHX:N1   | 86:1:4158:OHX:N2   | 2.67                     | 0.43              |
| 38:4:73:U:OP1      | 62:N6:24:SER:OG    | 2.28                     | 0.43              |
| 40:L3:261:MET:HE2  | 52:M6:64:PHE:CA    | 2.49                     | 0.43              |
| 41:L4:62:ALA:HB1   | 41:L4:76:ARG:C     | 2.43                     | 0.43              |
| 45:L8:152:LEU:HB3  | 45:L8:180:VAL:HG11 | 2.00                     | 0.43              |
| 46:L9:169:ASN:O    | 46:L9:170:LYS:HG2  | 2.19                     | 0.43              |
| 48:M1:17:LEU:HD21  | 48:M1:19:LEU:HD21  | 2.01                     | 0.43              |
| 49:M3:124:ILE:O    | 49:M3:124:ILE:HG12 | 2.18                     | 0.43              |
| 53:M7:26:PHE:HE1   | 53:M7:120:ASN:HA   | 1.83                     | 0.43              |
| 63:N7:84:ARG:HA    | 66:O0:62:LEU:HD21  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:O5:31:LEU:HD12  | 71:O5:31:LEU:HA    | 1.89                     | 0.43              |
| 78:Q2:63:LYS:HD2   | 78:Q2:87:ARG:CZ    | 2.49                     | 0.43              |
| 1:6:322:G:OP1      | 86:6:2107:OHX:N5   | 2.52                     | 0.43              |
| 1:6:521:A:O2'      | 26:d4:34:ASN:OD1   | 2.22                     | 0.43              |
| 1:6:636:A:O2'      | 1:6:637:C:H5'      | 2.19                     | 0.43              |
| 1:6:638:U:O2'      | 9:s7:101:LYS:HD3   | 2.19                     | 0.43              |
| 1:6:751:G:C2       | 1:6:752:A:C4       | 3.06                     | 0.43              |
| 1:6:804:A:C8       | 24:d2:107:SER:HA   | 2.54                     | 0.43              |
| 1:6:848:C:H2'      | 1:6:849:C:C6       | 2.54                     | 0.43              |
| 1:6:856:A:N6       | 9:s7:96:ARG:HB3    | 2.33                     | 0.43              |
| 1:6:1157:A:H2'     | 1:6:1160:A:N7      | 2.33                     | 0.43              |
| 1:6:1417:A:O2'     | 18:c6:128:LYS:HE3  | 2.18                     | 0.43              |
| 2:s0:65:ALA:O      | 2:s0:66:ALA:HB3    | 2.19                     | 0.43              |
| 5:s3:97:SER:O      | 5:s3:101:GLN:HG2   | 2.18                     | 0.43              |
| 9:s7:137:GLY:HA3   | 9:s7:153:LEU:HD12  | 2.01                     | 0.43              |
| 11:s9:162:SER:HA   | 11:s9:163:PRO:HD2  | 1.70                     | 0.43              |
| 15:c3:16:ILE:HG13  | 15:c3:62:GLN:NE2   | 2.32                     | 0.43              |
| 21:c9:16:ASN:OD1   | 21:c9:56:LYS:NZ    | 2.48                     | 0.43              |
| 22:d0:20:ILE:HD12  | 22:d0:100:VAL:HG21 | 2.01                     | 0.43              |
| 24:d2:55:ASP:CG    | 24:d2:57:ARG:HB2   | 2.43                     | 0.43              |
| 25:d3:56:LYS:NZ    | 25:d3:96:VAL:O     | 2.47                     | 0.43              |
| 36:5:118:U:C5      | 36:5:119:U:C4      | 3.06                     | 0.43              |
| 36:5:956:U:H2'     | 36:5:957:C:C6      | 2.53                     | 0.43              |
| 36:5:1080:A:OP1    | 42:l5:140:ARG:HB2  | 2.18                     | 0.43              |
| 36:5:1506:A:H1'    | 36:5:1848:G:C6     | 2.53                     | 0.43              |
| 36:5:1676:A:OP1    | 58:n2:13:LYS:NZ    | 2.52                     | 0.43              |
| 36:5:2183:A:O2'    | 39:l2:236:GLY:N    | 2.46                     | 0.43              |
| 36:5:2206:G:O2'    | 36:5:2207:A:H5'    | 2.19                     | 0.43              |
| 36:5:2816:G:C8     | 36:5:2869:U:H3'    | 2.53                     | 0.43              |
| 36:5:2840:C:H2'    | 36:5:2841:G:O4'    | 2.19                     | 0.43              |
| 36:5:2947:G:N3     | 40:l3:250:ALA:HB1  | 2.34                     | 0.43              |
| 36:5:3018:C:C4     | 36:5:3019:U:C4     | 3.07                     | 0.43              |
| 36:5:3245:A:H2     | 36:5:3246:G:N1     | 2.17                     | 0.43              |
| 86:5:4140:OHX:N4   | 86:5:4181:OHX:N1   | 2.67                     | 0.43              |
| 39:l2:180:LEU:HG   | 79:q3:26:VAL:HG21  | 2.01                     | 0.43              |
| 44:l7:116:PHE:HB2  | 44:l7:199:ASN:OD1  | 2.19                     | 0.43              |
| 45:l8:150:LEU:HD23 | 45:l8:176:PRO:HB2  | 2.01                     | 0.43              |
| 45:l8:195:SER:O    | 45:l8:197:VAL:N    | 2.52                     | 0.43              |
| 48:m1:26:SER:HB3   | 48:m1:63:GLU:HG2   | 2.00                     | 0.43              |
| 48:m1:92:ARG:O     | 48:m1:95:ASN:HB2   | 2.18                     | 0.43              |
| 51:m5:178:HIS:H    | 51:m5:178:HIS:HD1  | 1.66                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:n4:62:GLY:C     | 60:n4:63:ILE:HG13  | 2.44                     | 0.43              |
| 65:n9:23:LYS:HB3   | 65:n9:24:PRO:CD    | 2.48                     | 0.43              |
| 73:o7:84:SER:O     | 73:o7:85:LYS:HB2   | 2.18                     | 0.43              |
| 83:p1:29:UNK:C     | 83:p1:31:UNK:N     | 2.82                     | 0.43              |
| 1:2:179:A:H2'      | 1:2:180:A:O4'      | 2.19                     | 0.43              |
| 1:2:230:C:H2'      | 1:2:231:U:H5''     | 2.00                     | 0.43              |
| 1:2:321:C:N4       | 1:2:1667:A:OP1     | 2.51                     | 0.43              |
| 1:2:328:A:H2'      | 1:2:329:G:O4'      | 2.18                     | 0.43              |
| 1:2:712:G:H2'      | 1:2:713:A:O4'      | 2.18                     | 0.43              |
| 1:2:901:G:N2       | 16:C4:54:GLU:OE1   | 2.52                     | 0.43              |
| 1:2:1144:U:H2'     | 1:2:1145:U:C6      | 2.54                     | 0.43              |
| 1:2:1244:A:HO2'    | 1:2:1245:G:P       | 2.40                     | 0.43              |
| 1:2:1247:U:H5''    | 33:E1:94:LYS:O     | 2.18                     | 0.43              |
| 1:2:1604:U:C4      | 1:2:1605:G:N7      | 2.87                     | 0.43              |
| 3:S1:39:GLU:HB3    | 3:S1:73:LEU:O      | 2.18                     | 0.43              |
| 5:S3:163:PRO:O     | 5:S3:167:PHE:N     | 2.50                     | 0.43              |
| 6:S4:64:ILE:HG13   | 26:D4:18:LEU:HG    | 2.00                     | 0.43              |
| 7:S5:81:ARG:HD3    | 7:S5:82:PHE:CE2    | 2.54                     | 0.43              |
| 11:S9:93:LEU:O     | 11:S9:96:VAL:HG22  | 2.19                     | 0.43              |
| 18:C6:39:VAL:O     | 18:C6:40:GLU:C     | 2.62                     | 0.43              |
| 19:C7:13:SER:HA    | 19:C7:54:THR:HG22  | 2.00                     | 0.43              |
| 19:C7:23:LYS:H     | 34:SR:216:LYS:HE2  | 1.84                     | 0.43              |
| 21:C9:23:GLN:HG2   | 21:C9:55:TYR:CD2   | 2.54                     | 0.43              |
| 33:E1:89:LYS:HD2   | 33:E1:89:LYS:HA    | 1.76                     | 0.43              |
| 36:1:884:A:OP1     | 73:O7:5:THR:CG2    | 2.67                     | 0.43              |
| 36:1:1486:G:H21    | 70:O4:6:THR:HG22   | 1.83                     | 0.43              |
| 36:1:2242:A:H5''   | 39:L2:244:GLY:HA3  | 2.01                     | 0.43              |
| 36:1:2250:G:O2'    | 36:1:2251:G:H5'    | 2.19                     | 0.43              |
| 36:1:2718:U:OP2    | 86:1:3987:OHX:N3   | 2.51                     | 0.43              |
| 36:1:3049:A:C2     | 40:L3:75:ALA:HB2   | 2.54                     | 0.43              |
| 36:1:3174:A:C6     | 36:1:3175:U:C4     | 3.07                     | 0.43              |
| 36:1:3181:C:O2'    | 52:M6:164:SER:OG   | 2.29                     | 0.43              |
| 36:1:3353:G:O2'    | 36:1:3356:G:H5'    | 2.18                     | 0.43              |
| 42:L5:184:ASP:OD1  | 42:L5:187:THR:HG22 | 2.19                     | 0.43              |
| 42:L5:211:LEU:HD23 | 42:L5:211:LEU:HA   | 1.69                     | 0.43              |
| 44:L7:125:GLU:OE1  | 44:L7:128:LYS:HE3  | 2.19                     | 0.43              |
| 46:L9:2:LYS:HA     | 46:L9:60:GLY:O     | 2.18                     | 0.43              |
| 46:L9:4:ILE:HG22   | 56:N0:142:GLN:CD   | 2.43                     | 0.43              |
| 46:L9:45:PHE:CD1   | 46:L9:55:VAL:HG12  | 2.54                     | 0.43              |
| 48:M1:141:ARG:O    | 48:M1:145:LYS:HE2  | 2.18                     | 0.43              |
| 49:M3:126:PHE:CD1  | 49:M3:133:PRO:HG2  | 2.54                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:M6:18:ARG:O     | 52:M6:22:VAL:HG13  | 2.19                     | 0.43              |
| 56:N0:4:PHE:O      | 56:N0:100:VAL:HG22 | 2.18                     | 0.43              |
| 57:N1:27:LEU:HD22  | 57:N1:27:LEU:HA    | 1.80                     | 0.43              |
| 58:N2:19:VAL:O     | 58:N2:23:THR:OG1   | 2.18                     | 0.43              |
| 61:N5:49:LYS:O     | 61:N5:50:ALA:HB3   | 2.19                     | 0.43              |
| 62:N6:122:LYS:HE2  | 62:N6:122:LYS:HB3  | 1.83                     | 0.43              |
| 73:O7:69:HIS:O     | 73:O7:73:ARG:HG3   | 2.18                     | 0.43              |
| 74:O8:46:ARG:NH1   | 74:O8:47:GLY:O     | 2.51                     | 0.43              |
| 4:s2:111:VAL:O     | 4:s2:136:VAL:HA    | 2.19                     | 0.43              |
| 6:s4:23:LEU:O      | 6:s4:24:SER:OG     | 2.35                     | 0.43              |
| 15:c3:20:ARG:HD3   | 24:d2:56:HIS:CD2   | 2.54                     | 0.43              |
| 16:c4:18:ARG:HE    | 16:c4:18:ARG:HB2   | 1.65                     | 0.43              |
| 18:c6:116:LEU:HD23 | 18:c6:116:LEU:HA   | 1.78                     | 0.43              |
| 34:sR:232:TYR:OH   | 34:sR:265:LEU:HD22 | 2.19                     | 0.43              |
| 36:5:76:G:N7       | 49:m3:101:ARG:HB2  | 2.34                     | 0.43              |
| 36:5:612:U:OP1     | 43:l6:21:THR:HB    | 2.19                     | 0.43              |
| 36:5:1806:A:H2'    | 36:5:1807:G:O4'    | 2.19                     | 0.43              |
| 36:5:1876:U:C5'    | 36:5:1876:U:C6     | 3.01                     | 0.43              |
| 36:5:2709:C:H2'    | 36:5:2710:C:C6     | 2.54                     | 0.43              |
| 36:5:2947:G:N2     | 36:5:2948:C:C2     | 2.86                     | 0.43              |
| 36:5:3275:U:O3'    | 36:5:3276:G:C2     | 2.71                     | 0.43              |
| 36:5:3362:A:H2'    | 36:5:3363:U:O4'    | 2.19                     | 0.43              |
| 40:l3:233:TRP:CD1  | 40:l3:265:ALA:HB1  | 2.54                     | 0.43              |
| 43:l6:90:LYS:HE3   | 43:l6:90:LYS:HB2   | 1.68                     | 0.43              |
| 49:m3:18:TRP:CD1   | 49:m3:18:TRP:H     | 2.36                     | 0.43              |
| 52:m6:14:HIS:O     | 52:m6:41:LEU:HD12  | 2.18                     | 0.43              |
| 53:m7:4:TYR:CZ     | 53:m7:18:ARG:HG3   | 2.53                     | 0.43              |
| 54:m8:165:ILE:HD12 | 54:m8:173:GLU:CD   | 2.44                     | 0.43              |
| 57:n1:71:SER:HB3   | 57:n1:91:LEU:O     | 2.18                     | 0.43              |
| 70:o4:22:VAL:CG1   | 70:o4:30:LEU:HD13  | 2.49                     | 0.43              |
| 72:o6:55:ARG:O     | 72:o6:58:ILE:HD13  | 2.19                     | 0.43              |
| 1:2:485:A:H2'      | 1:2:486:G:O4'      | 2.18                     | 0.43              |
| 1:2:1222:C:H2'     | 1:2:1223:A:O4'     | 2.19                     | 0.43              |
| 1:2:1682:U:O2'     | 1:2:1683:C:H5'     | 2.19                     | 0.43              |
| 86:2:2084:OHX:N6   | 86:2:2086:OHX:N2   | 2.66                     | 0.43              |
| 3:S1:61:LEU:HG     | 3:S1:64:ARG:HH21   | 1.84                     | 0.43              |
| 3:S1:140:ILE:O     | 3:S1:210:ILE:HA    | 2.18                     | 0.43              |
| 5:S3:142:LEU:HD12  | 5:S3:142:LEU:HA    | 1.86                     | 0.43              |
| 10:S8:114:GLU:HG2  | 10:S8:120:THR:HA   | 2.01                     | 0.43              |
| 11:S9:163:PRO:C    | 11:S9:165:GLY:N    | 2.77                     | 0.43              |
| 16:C4:84:ARG:HG2   | 16:C4:85:ALA:O     | 2.19                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:C5:15:HIS:HB3   | 17:C5:22:LEU:CD2   | 2.48                     | 0.43              |
| 19:C7:33:ARG:HG3   | 34:SR:127:ARG:NH1  | 2.34                     | 0.43              |
| 19:C7:81:LYS:HB2   | 19:C7:81:LYS:HE3   | 1.70                     | 0.43              |
| 21:C9:66:TYR:HA    | 21:C9:124:ILE:HB   | 2.00                     | 0.43              |
| 22:D0:104:THR:HG21 | 22:D0:116:VAL:HG21 | 1.99                     | 0.43              |
| 23:D1:36:VAL:O     | 23:D1:51:VAL:N     | 2.51                     | 0.43              |
| 24:D2:17:ALA:HB2   | 24:D2:25:VAL:CG1   | 2.47                     | 0.43              |
| 28:D6:4:LYS:O      | 28:D6:4:LYS:HG3    | 2.18                     | 0.43              |
| 34:SR:232:TYR:CE1  | 34:SR:234:LEU:HD11 | 2.54                     | 0.43              |
| 36:1:246:U:H2'     | 36:1:247:C:C6      | 2.53                     | 0.43              |
| 36:1:1355:A:H4'    | 36:1:1356:U:O5'    | 2.17                     | 0.43              |
| 36:1:2703:A:OP2    | 42:L5:23:ARG:NH1   | 2.48                     | 0.43              |
| 36:1:2960:C:H2'    | 36:1:2961:G:H8     | 1.82                     | 0.43              |
| 36:1:3383:G:H2'    | 36:1:3384:U:H6     | 1.83                     | 0.43              |
| 37:3:58:C:H2'      | 37:3:59:U:H6       | 1.84                     | 0.43              |
| 42:L5:177:GLU:H    | 42:L5:177:GLU:HG3  | 1.61                     | 0.43              |
| 46:L9:88:TYR:CE2   | 46:L9:184:LYS:HE2  | 2.53                     | 0.43              |
| 51:M5:11:GLN:HG2   | 51:M5:44:ARG:HH21  | 1.82                     | 0.43              |
| 52:M6:127:LEU:HD22 | 56:N0:156:VAL:HG23 | 2.01                     | 0.43              |
| 60:N4:57:LYS:HB2   | 60:N4:57:LYS:HE3   | 1.82                     | 0.43              |
| 61:N5:57:LEU:HA    | 61:N5:57:LEU:HD12  | 1.79                     | 0.43              |
| 1:6:94:U:H2'       | 1:6:95:G:O4'       | 2.19                     | 0.43              |
| 1:6:470:A:H5''     | 1:6:470:A:H8       | 1.83                     | 0.43              |
| 1:6:566:C:O2       | 80:e0:13:LYS:HE2   | 2.19                     | 0.43              |
| 1:6:837:G:H2'      | 1:6:838:G:C8       | 2.54                     | 0.43              |
| 1:6:1317:C:H2'     | 1:6:1318:G:O4'     | 2.17                     | 0.43              |
| 1:6:1429:G:H2'     | 1:6:1430:U:H6      | 1.82                     | 0.43              |
| 1:6:1649:G:H2'     | 1:6:1650:U:C6      | 2.54                     | 0.43              |
| 5:s3:8:LYS:HG2     | 22:d0:63:LEU:HD21  | 2.00                     | 0.43              |
| 19:c7:26:LEU:HD22  | 19:c7:59:LYS:HA    | 2.00                     | 0.43              |
| 19:c7:34:LEU:HD23  | 19:c7:34:LEU:HA    | 1.85                     | 0.43              |
| 20:c8:119:ILE:HD12 | 20:c8:119:ILE:HA   | 1.56                     | 0.43              |
| 29:d7:61:THR:OG1   | 29:d7:62:ILE:N     | 2.51                     | 0.43              |
| 30:d8:44:VAL:HG21  | 30:d8:48:VAL:CG2   | 2.49                     | 0.43              |
| 33:e1:144:CYS:C    | 33:e1:146:SER:N    | 2.77                     | 0.43              |
| 36:5:947:G:C5'     | 68:o2:55:ILE:HB    | 2.49                     | 0.43              |
| 36:5:1226:G:H2'    | 36:5:1227:C:C6     | 2.53                     | 0.43              |
| 36:5:1565:G:N2     | 36:5:1566:A:H1'    | 2.34                     | 0.43              |
| 36:5:2192:C:H2'    | 36:5:2193:U:O4'    | 2.19                     | 0.43              |
| 36:5:2573:G:H3'    | 36:5:2574:G:H5''   | 2.00                     | 0.43              |
| 36:5:2799:A:H1'    | 64:n8:42:ARG:HH21  | 1.82                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:5:4034:OHX:N2   | 86:5:4117:OHX:N4   | 2.66                     | 0.43              |
| 40:13:139:GLN:C    | 40:13:141:GLY:H    | 2.27                     | 0.43              |
| 40:13:331:ASN:OD1  | 40:13:331:ASN:N    | 2.46                     | 0.43              |
| 43:16:52:VAL:CG1   | 43:16:65:ILE:HG13  | 2.49                     | 0.43              |
| 45:18:156:ASP:O    | 45:18:183:LYS:HE3  | 2.18                     | 0.43              |
| 45:18:242:ALA:HA   | 45:18:245:LYS:HD3  | 1.99                     | 0.43              |
| 53:m7:105:LYS:HB3  | 53:m7:107:LEU:HD13 | 2.00                     | 0.43              |
| 1:2:473:A:H4'      | 1:2:768:C:O2       | 2.19                     | 0.43              |
| 1:2:885:G:H2'      | 1:2:886:U:C6       | 2.53                     | 0.43              |
| 1:2:1015:U:H5''    | 1:2:1016:C:OP2     | 2.18                     | 0.43              |
| 1:2:1561:U:H4'     | 1:2:1599:C:H4'     | 2.01                     | 0.43              |
| 1:2:1600:A:O2'     | 1:2:1602:C:N4      | 2.51                     | 0.43              |
| 1:2:1767:G:OP2     | 1:2:1770:U:O2'     | 2.28                     | 0.43              |
| 2:S0:66:ALA:HB2    | 23:D1:37:ALA:HB2   | 2.01                     | 0.43              |
| 3:S1:172:LEU:O     | 3:S1:176:VAL:HG23  | 2.19                     | 0.43              |
| 6:S4:71:LYS:HA     | 6:S4:76:VAL:O      | 2.19                     | 0.43              |
| 6:S4:194:THR:OG1   | 6:S4:195:ILE:N     | 2.50                     | 0.43              |
| 8:S6:58:LYS:C      | 8:S6:60:GLY:H      | 2.27                     | 0.43              |
| 10:S8:122:GLY:O    | 86:S8:302:OHX:N6   | 2.51                     | 0.43              |
| 11:S9:110:GLN:NE2  | 11:S9:122:VAL:O    | 2.51                     | 0.43              |
| 33:E1:109:ASP:HB2  | 33:E1:113:LYS:HD3  | 2.00                     | 0.43              |
| 33:E1:127:GLY:C    | 33:E1:129:GLY:H    | 2.22                     | 0.43              |
| 34:SR:29:GLN:H     | 34:SR:29:GLN:HG2   | 1.54                     | 0.43              |
| 34:SR:240:VAL:HG22 | 34:SR:256:THR:HG22 | 2.00                     | 0.43              |
| 36:1:743:C:O2      | 54:M8:141:ARG:HD2  | 2.18                     | 0.43              |
| 36:1:860:G:C6      | 39:L2:181:LYS:HB3  | 2.54                     | 0.43              |
| 36:1:1615:C:H2'    | 36:1:1616:U:H6     | 1.84                     | 0.43              |
| 36:1:1621:A:H2'    | 36:1:1622:U:C6     | 2.54                     | 0.43              |
| 36:1:1845:G:H5''   | 36:1:1845:G:H8     | 1.84                     | 0.43              |
| 36:1:1925:U:O2'    | 36:1:1927:G:N7     | 2.50                     | 0.43              |
| 36:1:2529:A:C2     | 36:1:2582:C:C2     | 3.06                     | 0.43              |
| 36:1:2544:U:H2'    | 36:1:2545:C:H6     | 1.84                     | 0.43              |
| 44:L7:136:TYR:C    | 44:L7:236:ILE:HD13 | 2.44                     | 0.43              |
| 45:L8:65:LEU:HD12  | 51:M5:25:VAL:HG13  | 1.99                     | 0.43              |
| 48:M1:171:VAL:HG13 | 48:M1:172:LEU:N    | 2.34                     | 0.43              |
| 62:N6:115:ARG:O    | 62:N6:119:ILE:HG13 | 2.19                     | 0.43              |
| 70:O4:67:LYS:HA    | 70:O4:70:LYS:HE3   | 2.01                     | 0.43              |
| 78:Q2:14:GLY:O     | 78:Q2:16:THR:N     | 2.52                     | 0.43              |
| 1:6:138:A:H62      | 1:6:266:A:H61      | 1.66                     | 0.43              |
| 1:6:727:U:H2'      | 1:6:728:U:C6       | 2.53                     | 0.43              |
| 1:6:1085:G:N2      | 1:6:1088:A:OP2     | 2.46                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:1198:G:OP1     | 1:6:1199:G:H1'     | 2.18                     | 0.43              |
| 1:6:1228:G:OP2     | 1:6:1228:G:H4'     | 2.19                     | 0.43              |
| 1:6:1518:C:OP2     | 86:6:2143:OHX:N1   | 2.52                     | 0.43              |
| 1:6:1533:C:H4'     | 1:6:1539:G:C6      | 2.53                     | 0.43              |
| 3:s1:54:LEU:HD23   | 3:s1:54:LEU:HA     | 1.86                     | 0.43              |
| 13:c1:36:LYS:HE2   | 13:c1:59:PRO:O     | 2.19                     | 0.43              |
| 23:d1:74:GLN:HE21  | 23:d1:74:GLN:HB3   | 1.70                     | 0.43              |
| 26:d4:53:ASP:OD1   | 26:d4:96:LEU:HD21  | 2.18                     | 0.43              |
| 80:e0:14:VAL:HA    | 80:e0:17:GLN:HG2   | 2.00                     | 0.43              |
| 34:sR:100:TYR:HD2  | 34:sR:100:TYR:HA   | 1.73                     | 0.43              |
| 36:5:48:A:O4'      | 36:5:50:U:C6       | 2.72                     | 0.43              |
| 36:5:291:C:P       | 51:m5:68:ARG:HH11  | 2.42                     | 0.43              |
| 36:5:541:U:O4      | 86:5:4013:OHX:N3   | 2.52                     | 0.43              |
| 36:5:825:U:O5'     | 36:5:825:U:H6      | 2.01                     | 0.43              |
| 36:5:1370:G:H5''   | 64:n8:18:GLY:O     | 2.19                     | 0.43              |
| 36:5:1500:G:H2'    | 36:5:1501:U:O4'    | 2.19                     | 0.43              |
| 36:5:2287:C:C5     | 36:5:2298:U:C2     | 3.07                     | 0.43              |
| 36:5:2425:G:H2'    | 36:5:2426:U:C6     | 2.53                     | 0.43              |
| 36:5:2618:G:C5     | 47:m0:115:MET:HB3  | 2.53                     | 0.43              |
| 36:5:3242:G:H21    | 36:5:3245:A:H5''   | 1.83                     | 0.43              |
| 86:5:4093:OHX:N6   | 86:5:4199:OHX:N2   | 2.66                     | 0.43              |
| 38:8:142:C:H2'     | 38:8:143:U:C6      | 2.54                     | 0.43              |
| 39:12:15:ILE:HD12  | 39:12:15:ILE:HA    | 1.71                     | 0.43              |
| 39:12:149:ARG:HH22 | 39:12:253:GLN:CB   | 2.32                     | 0.43              |
| 41:14:140:HIS:CG   | 41:14:247:PHE:HB2  | 2.54                     | 0.43              |
| 42:15:95:TRP:CD1   | 42:15:95:TRP:C     | 2.97                     | 0.43              |
| 53:m7:28:ASN:O     | 53:m7:32:THR:HG23  | 2.19                     | 0.43              |
| 53:m7:112:LEU:HD12 | 53:m7:112:LEU:HA   | 1.76                     | 0.43              |
| 54:m8:2:GLY:O      | 54:m8:3:ILE:HD13   | 2.19                     | 0.43              |
| 61:n5:24:LEU:HB3   | 61:n5:25:LYS:H     | 1.63                     | 0.43              |
| 61:n5:105:VAL:HG21 | 61:n5:135:ILE:HG13 | 2.01                     | 0.43              |
| 67:o1:44:MET:HE2   | 67:o1:44:MET:HB2   | 1.48                     | 0.43              |
| 70:o4:74:ARG:HG2   | 70:o4:75:ALA:H     | 1.83                     | 0.43              |
| 71:o5:31:LEU:HD12  | 71:o5:31:LEU:HA    | 1.83                     | 0.43              |
| 74:o8:46:ARG:NH1   | 74:o8:47:GLY:O     | 2.51                     | 0.43              |
| 82:p0:10:GLU:O     | 82:p0:13:ALA:HB3   | 2.17                     | 0.43              |
| 82:p0:97:LYS:O     | 82:p0:101:VAL:HG23 | 2.19                     | 0.43              |
| 1:2:72:A:C2        | 1:2:73:U:C4        | 3.06                     | 0.43              |
| 1:2:867:G:P        | 15:C3:3:ARG:NH1    | 2.92                     | 0.43              |
| 4:S2:227:PRO:HA    | 4:S2:230:TRP:CD1   | 2.54                     | 0.43              |
| 7:S5:37:GLN:NE2    | 18:C6:53:LEU:HD13  | 2.33                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:S7:43:PHE:HB2   | 9:S7:61:PHE:O     | 2.19                     | 0.43              |
| 9:S7:46:ILE:HG12  | 9:S7:60:ILE:HA    | 2.00                     | 0.43              |
| 19:C7:21:TYR:HA   | 19:C7:58:MET:HE1  | 2.00                     | 0.43              |
| 24:D2:24:GLN:OE1  | 29:D7:4:VAL:HA    | 2.19                     | 0.43              |
| 27:D5:43:ASP:N    | 27:D5:46:LYS:HD2  | 2.33                     | 0.43              |
| 28:D6:87:ARG:NH2  | 28:D6:94:ASN:O    | 2.39                     | 0.43              |
| 31:D9:21:CYS:HB2  | 31:D9:39:CYS:HB3  | 2.01                     | 0.43              |
| 34:SR:147:HIS:CD2 | 34:SR:179:LYS:HD2 | 2.53                     | 0.43              |
| 35:SM:61:ILE:H    | 35:SM:61:ILE:HG13 | 1.61                     | 0.43              |
| 36:1:291:C:OP2    | 51:M5:128:LYS:NZ  | 2.52                     | 0.43              |
| 36:1:1237:G:H2'   | 36:1:1237:G:N3    | 2.34                     | 0.43              |
| 36:1:1487:G:H1    | 36:1:1855:U:H3    | 1.67                     | 0.43              |
| 36:1:1759:C:H2'   | 36:1:1760:A:O4'   | 2.19                     | 0.43              |
| 36:1:2192:C:H2'   | 36:1:2193:U:O4'   | 2.18                     | 0.43              |
| 36:1:2208:A:C2    | 86:1:4047:OHX:N6  | 2.87                     | 0.43              |
| 36:1:2284:C:H5''  | 36:1:2285:C:OP2   | 2.18                     | 0.43              |
| 36:1:2939:G:C2'   | 36:1:2940:A:H5'   | 2.48                     | 0.43              |
| 36:1:3116:G:N3    | 36:1:3116:G:H2'   | 2.34                     | 0.43              |
| 36:1:3316:A:OP1   | 36:1:3318:G:N2    | 2.52                     | 0.43              |
| 40:L3:3:HIS:O     | 40:L3:4:ARG:C     | 2.62                     | 0.43              |
| 41:L4:3:ARG:HH21  | 41:L4:3:ARG:HG2   | 1.84                     | 0.43              |
| 42:L5:41:LYS:HD2  | 42:L5:41:LYS:HA   | 1.62                     | 0.43              |
| 48:M1:54:VAL:O    | 48:M1:56:THR:N    | 2.49                     | 0.43              |
| 48:M1:94:ARG:C    | 48:M1:96:PHE:N    | 2.75                     | 0.43              |
| 52:M6:23:VAL:HG11 | 52:M6:84:LEU:HD11 | 2.01                     | 0.43              |
| 52:M6:98:ALA:O    | 52:M6:101:ARG:HB2 | 2.18                     | 0.43              |
| 66:O0:78:GLY:HA2  | 66:O0:87:VAL:HG13 | 2.01                     | 0.43              |
| 72:O6:40:VAL:O    | 72:O6:44:VAL:HG23 | 2.19                     | 0.43              |
| 74:O8:78:LEU:HA   | 74:O8:78:LEU:HD13 | 1.69                     | 0.43              |
| 1:6:225:A:O2'     | 1:6:226:A:H5'     | 2.19                     | 0.43              |
| 1:6:639:U:OP1     | 9:s7:112:ARG:NH2  | 2.52                     | 0.43              |
| 1:6:788:A:OP1     | 6:s4:106:LYS:NZ   | 2.44                     | 0.43              |
| 1:6:1397:U:C5     | 1:6:1399:C:C2     | 3.07                     | 0.43              |
| 1:6:1477:G:O2'    | 21:c9:47:PRO:HA   | 2.19                     | 0.43              |
| 1:6:1568:C:H6     | 1:6:1568:C:H2'    | 1.57                     | 0.43              |
| 1:6:1628:U:H2'    | 1:6:1629:G:C8     | 2.54                     | 0.43              |
| 5:s3:212:LYS:HD2  | 5:s3:212:LYS:HA   | 1.89                     | 0.43              |
| 8:s6:169:TYR:HE2  | 8:s6:171:LYS:HD2  | 1.82                     | 0.43              |
| 10:s8:59:ARG:O    | 10:s8:60:ILE:HG13 | 2.19                     | 0.43              |
| 13:c1:5:LEU:HD23  | 13:c1:7:VAL:HA    | 2.01                     | 0.43              |
| 13:c1:30:ARG:H    | 13:c1:30:ARG:HG2  | 1.54                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:d2:114:GLU:HG2  | 24:d2:118:ARG:NH2 | 2.32                     | 0.43              |
| 25:d3:92:CYS:HG    | 25:d3:136:TRP:CD1 | 2.37                     | 0.43              |
| 36:5:155:G:H1'     | 72:o6:26:ILE:HD13 | 2.01                     | 0.43              |
| 36:5:171:G:N2      | 36:5:248:U:O2     | 2.52                     | 0.43              |
| 36:5:314:U:H2'     | 36:5:315:C:C6     | 2.54                     | 0.43              |
| 36:5:1015:U:P      | 36:5:1016:C:OP1   | 2.77                     | 0.43              |
| 36:5:1258:U:O2     | 36:5:1260:A:C8    | 2.71                     | 0.43              |
| 36:5:1382:G:OP2    | 41:l4:188:ARG:NH1 | 2.52                     | 0.43              |
| 36:5:1677:G:OP1    | 58:n2:100:THR:HA  | 2.18                     | 0.43              |
| 36:5:1796:G:O6     | 86:5:4225:OHX:N5  | 2.51                     | 0.43              |
| 36:5:1807:G:C6     | 36:5:1808:G:N1    | 2.86                     | 0.43              |
| 36:5:1895:A:O2'    | 36:5:3053:G:H4'   | 2.18                     | 0.43              |
| 36:5:2985:C:H2'    | 36:5:2986:U:C6    | 2.54                     | 0.43              |
| 86:5:4034:OHX:N5   | 86:5:4117:OHX:N3  | 2.67                     | 0.43              |
| 39:l2:77:ILE:HD12  | 39:l2:128:ARG:HB3 | 2.01                     | 0.43              |
| 39:l2:177:LYS:HB2  | 79:q3:29:LEU:HD13 | 2.01                     | 0.43              |
| 41:l4:145:ILE:O    | 86:l4:402:OHX:N4  | 2.52                     | 0.43              |
| 56:n0:155:ARG:HH21 | 56:n0:172:TYR:H   | 1.66                     | 0.43              |
| 57:n1:39:ILE:HD12  | 57:n1:102:ARG:NE  | 2.34                     | 0.43              |
| 59:n3:13:ILE:HD11  | 59:n3:81:GLN:OE1  | 2.18                     | 0.43              |
| 62:n6:39:LEU:HD22  | 62:n6:43:TYR:HE2  | 1.83                     | 0.43              |
| 66:o0:13:LYS:O     | 66:o0:17:VAL:HG23 | 2.19                     | 0.43              |
| 66:o0:78:GLY:HA2   | 66:o0:87:VAL:HG13 | 1.99                     | 0.43              |
| 67:o1:46:THR:HG23  | 67:o1:47:ASP:H    | 1.82                     | 0.43              |
| 68:o2:31:ASN:OD1   | 68:o2:31:ASN:N    | 2.44                     | 0.43              |
| 72:o6:25:LYS:HG3   | 72:o6:28:TYR:CE2  | 2.53                     | 0.43              |
| 73:o7:29:VAL:O     | 73:o7:32:LYS:HD3  | 2.19                     | 0.43              |
| 77:q1:15:ARG:HG3   | 77:q1:15:ARG:NH1  | 2.34                     | 0.43              |
| 82:p0:63:ILE:HG21  | 82:p0:77:LEU:HD21 | 2.01                     | 0.43              |
| 82:p0:67:LEU:HD11  | 82:p0:74:GLU:HB2  | 2.01                     | 0.43              |
| 1:2:300:A:O2'      | 1:2:301:A:H5'     | 2.19                     | 0.42              |
| 1:2:682:C:H2'      | 1:2:683:C:O4'     | 2.19                     | 0.42              |
| 1:2:693:U:H5'      | 1:2:694:U:C5'     | 2.48                     | 0.42              |
| 2:S0:179:ARG:O     | 2:S0:183:ARG:HG3  | 2.19                     | 0.42              |
| 3:S1:181:LEU:H     | 3:S1:181:LEU:HD13 | 1.84                     | 0.42              |
| 8:S6:98:ARG:HD3    | 8:S6:99:GLY:N     | 2.34                     | 0.42              |
| 10:S8:114:GLU:CD   | 10:S8:120:THR:HA  | 2.44                     | 0.42              |
| 28:D6:40:ALA:HB3   | 28:D6:69:ASN:ND2  | 2.34                     | 0.42              |
| 34:SR:201:THR:CB   | 34:SR:242:SER:HA  | 2.49                     | 0.42              |
| 36:1:535:G:C6      | 36:1:555:U:N3     | 2.86                     | 0.42              |
| 36:1:612:U:H2'     | 36:1:613:G:C8     | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:1177:G:H5'    | 69:O3:18:ARG:NH1   | 2.34                     | 0.42              |
| 36:1:1245:A:N6     | 36:1:1272:C:O2'    | 2.52                     | 0.42              |
| 36:1:1949:G:OP2    | 55:M9:135:LYS:NZ   | 2.52                     | 0.42              |
| 36:1:2427:U:H2'    | 36:1:2428:U:C6     | 2.53                     | 0.42              |
| 36:1:2572:C:O2'    | 36:1:2573:G:C8     | 2.72                     | 0.42              |
| 36:1:3215:A:C5'    | 50:M4:121:MET:HE1  | 2.49                     | 0.42              |
| 37:3:67:G:H2'      | 37:3:68:C:O4'      | 2.20                     | 0.42              |
| 37:3:73:C:C5       | 56:N0:13:ARG:NH1   | 2.87                     | 0.42              |
| 40:L3:91:GLY:O     | 40:L3:102:LEU:HD23 | 2.19                     | 0.42              |
| 40:L3:221:THR:HB   | 40:L3:273:HIS:H    | 1.84                     | 0.42              |
| 41:L4:82:THR:O     | 41:L4:82:THR:OG1   | 2.35                     | 0.42              |
| 41:L4:150:LEU:HD11 | 41:L4:172:VAL:HG13 | 2.01                     | 0.42              |
| 41:L4:193:LYS:HB2  | 41:L4:193:LYS:HE3  | 1.60                     | 0.42              |
| 45:L8:230:LYS:HD2  | 45:L8:230:LYS:HA   | 1.71                     | 0.42              |
| 52:M6:56:ASP:O     | 52:M6:59:ARG:HG2   | 2.19                     | 0.42              |
| 54:M8:99:THR:HB    | 54:M8:100:THR:H    | 1.43                     | 0.42              |
| 56:N0:42:TRP:NE1   | 56:N0:53:LYS:HG3   | 2.34                     | 0.42              |
| 59:N3:102:ILE:HG13 | 59:N3:110:LYS:HB3  | 2.01                     | 0.42              |
| 77:Q1:9:ARG:HH11   | 77:Q1:9:ARG:HG3    | 1.84                     | 0.42              |
| 1:6:29:U:H2'       | 1:6:30:G:H8        | 1.84                     | 0.42              |
| 1:6:357:G:OP2      | 86:6:2075:OHX:N6   | 2.51                     | 0.42              |
| 1:6:876:G:H1'      | 1:6:944:A:O4'      | 2.19                     | 0.42              |
| 1:6:1228:G:N3      | 1:6:1228:G:H2'     | 2.34                     | 0.42              |
| 1:6:1334:U:H2'     | 1:6:1335:U:C6      | 2.54                     | 0.42              |
| 3:s1:57:ALA:O      | 3:s1:61:LEU:HB2    | 2.19                     | 0.42              |
| 3:s1:133:TYR:CE2   | 3:s1:181:LEU:HD12  | 2.53                     | 0.42              |
| 3:s1:232:HIS:HB3   | 3:s1:233:GLY:H     | 1.47                     | 0.42              |
| 6:s4:89:VAL:O      | 6:s4:99:PHE:O      | 2.37                     | 0.42              |
| 6:s4:244:ILE:HD12  | 6:s4:244:ILE:HA    | 1.77                     | 0.42              |
| 8:s6:68:LEU:HD13   | 8:s6:68:LEU:HA     | 1.50                     | 0.42              |
| 9:s7:131:PHE:CD2   | 9:s7:132:PRO:HD3   | 2.54                     | 0.42              |
| 11:s9:167:ALA:O    | 11:s9:168:ARG:HB2  | 2.17                     | 0.42              |
| 19:c7:104:ASN:O    | 19:c7:106:THR:HG22 | 2.19                     | 0.42              |
| 19:c7:105:GLN:O    | 19:c7:109:LEU:N    | 2.51                     | 0.42              |
| 24:d2:23:ARG:CB    | 29:d7:4:VAL:HG12   | 2.49                     | 0.42              |
| 80:e0:18:THR:HA    | 80:e0:19:PRO:HD2   | 1.89                     | 0.42              |
| 35:sM:43:ASP:HA    | 35:sM:44:PRO:HD3   | 1.66                     | 0.42              |
| 36:5:98:G:OP1      | 49:m3:16:LYS:NZ    | 2.52                     | 0.42              |
| 36:5:422:A:N1      | 36:5:2362:C:O2'    | 2.41                     | 0.42              |
| 36:5:817:A:O2'     | 73:o7:11:ARG:HG2   | 2.18                     | 0.42              |
| 36:5:945:C:H2'     | 36:5:946:U:H6      | 1.83                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:1231:A:H5''   | 36:5:1232:C:H5'    | 1.99                     | 0.42              |
| 36:5:1258:U:H4'    | 82:p0:42:ARG:CZ    | 2.49                     | 0.42              |
| 36:5:1434:G:H5''   | 36:5:1437:C:C5     | 2.53                     | 0.42              |
| 36:5:3157:U:H3'    | 36:5:3158:G:H4'    | 2.01                     | 0.42              |
| 38:8:123:G:OP2     | 86:8:222:OHX:N6    | 2.52                     | 0.42              |
| 42:l5:126:GLU:HA   | 42:l5:196:ARG:HD2  | 1.99                     | 0.42              |
| 48:m1:12:LEU:HD12  | 48:m1:162:TRP:CG   | 2.54                     | 0.42              |
| 81:m2:152:UNK:C    | 81:m2:154:UNK:N    | 2.81                     | 0.42              |
| 52:m6:78:ARG:NH1   | 52:m6:78:ARG:HG3   | 2.33                     | 0.42              |
| 52:m6:156:LEU:HD23 | 52:m6:156:LEU:HA   | 1.64                     | 0.42              |
| 54:m8:86:THR:CG2   | 54:m8:105:ARG:HB2  | 2.49                     | 0.42              |
| 57:n1:17:ARG:HG2   | 57:n1:17:ARG:HH11  | 1.83                     | 0.42              |
| 57:n1:104:GLU:HG3  | 57:n1:105:PHE:N    | 2.33                     | 0.42              |
| 58:n2:43:VAL:O     | 58:n2:44:GLU:C     | 2.62                     | 0.42              |
| 1:2:145:A:O2'      | 1:2:146:U:O5'      | 2.34                     | 0.42              |
| 1:2:229:U:H2'      | 1:2:230:C:H6       | 1.83                     | 0.42              |
| 1:2:480:G:N2       | 1:2:509:G:H1'      | 2.34                     | 0.42              |
| 1:2:533:U:C4'      | 26:D4:33:ALA:HB2   | 2.49                     | 0.42              |
| 1:2:542:A:O2'      | 1:2:543:C:O5'      | 2.37                     | 0.42              |
| 1:2:698:U:O4       | 86:2:2097:OHX:N3   | 2.51                     | 0.42              |
| 1:2:699:U:OP2      | 1:2:733:A:N6       | 2.52                     | 0.42              |
| 1:2:732:G:N3       | 1:2:732:G:H2'      | 2.34                     | 0.42              |
| 1:2:1186:U:O4      | 1:2:1200:G:N2      | 2.45                     | 0.42              |
| 2:S0:32:HIS:ND1    | 2:S0:32:HIS:O      | 2.52                     | 0.42              |
| 5:S3:113:LEU:HD23  | 5:S3:113:LEU:HA    | 1.84                     | 0.42              |
| 10:S8:38:ILE:CD1   | 10:S8:80:GLY:HA2   | 2.49                     | 0.42              |
| 10:S8:58:LEU:O     | 10:S8:59:ARG:HB2   | 2.18                     | 0.42              |
| 16:C4:23:PHE:HE2   | 16:C4:91:THR:HG21  | 1.84                     | 0.42              |
| 17:C5:85:ILE:HA    | 17:C5:89:MET:SD    | 2.59                     | 0.42              |
| 21:C9:93:HIS:O     | 21:C9:94:ILE:HD12  | 2.19                     | 0.42              |
| 32:E0:41:THR:HA    | 32:E0:45:VAL:HB    | 2.00                     | 0.42              |
| 34:SR:109:ASP:HB2  | 34:SR:127:ARG:HD2  | 2.00                     | 0.42              |
| 34:SR:123:ILE:H    | 34:SR:123:ILE:HG13 | 1.70                     | 0.42              |
| 34:SR:269:TYR:CE2  | 34:SR:271:VAL:HG22 | 2.54                     | 0.42              |
| 36:1:112:U:O2'     | 36:1:113:C:P       | 2.77                     | 0.42              |
| 36:1:634:C:H5'     | 69:O3:21:ARG:O     | 2.19                     | 0.42              |
| 36:1:810:A:H2'     | 36:1:811:U:C6      | 2.55                     | 0.42              |
| 36:1:1355:A:H5'    | 36:1:1357:G:H1'    | 2.01                     | 0.42              |
| 36:1:1483:G:C8     | 36:1:1485:G:C8     | 3.07                     | 0.42              |
| 36:1:2094:C:H2'    | 36:1:2095:G:C8     | 2.53                     | 0.42              |
| 36:1:2295:A:H5'    | 59:N3:61:THR:HG21  | 2.01                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:3165:A:H61    | 36:1:3285:C:H42    | 1.66                     | 0.42              |
| 37:3:113:C:H2'     | 37:3:114:U:O4'     | 2.19                     | 0.42              |
| 41:L4:271:LYS:HB2  | 41:L4:274:TYR:HB3  | 2.01                     | 0.42              |
| 42:L5:58:LYS:HD2   | 42:L5:93:THR:OG1   | 2.19                     | 0.42              |
| 45:L8:25:PRO:HB2   | 45:L8:26:LEU:H     | 1.49                     | 0.42              |
| 45:L8:84:ARG:HB3   | 45:L8:84:ARG:CZ    | 2.49                     | 0.42              |
| 45:L8:220:ALA:HA   | 45:L8:224:ASP:OD2  | 2.19                     | 0.42              |
| 49:M3:94:GLY:HA3   | 71:O5:116:TYR:CZ   | 2.54                     | 0.42              |
| 52:M6:12:LYS:O     | 56:N0:167:ARG:NH2  | 2.34                     | 0.42              |
| 52:M6:113:ASP:OD2  | 52:M6:113:ASP:N    | 2.52                     | 0.42              |
| 57:N1:14:MET:HE2   | 57:N1:14:MET:HB3   | 1.61                     | 0.42              |
| 59:N3:86:ARG:HB2   | 59:N3:92:PHE:CE1   | 2.53                     | 0.42              |
| 61:N5:106:ASP:HB2  | 61:N5:130:TYR:CE1  | 2.54                     | 0.42              |
| 62:N6:37:LYS:H     | 62:N6:37:LYS:CD    | 2.31                     | 0.42              |
| 65:N9:54:LEU:HD23  | 65:N9:54:LEU:HA    | 1.87                     | 0.42              |
| 72:O6:74:LYS:HD2   | 72:O6:80:PHE:HD2   | 1.83                     | 0.42              |
| 1:6:755:A:O2'      | 1:6:756:A:OP1      | 2.37                     | 0.42              |
| 1:6:1152:A:O2'     | 1:6:1153:G:H5'     | 2.18                     | 0.42              |
| 1:6:1425:A:O2'     | 1:6:1426:C:H5'     | 2.19                     | 0.42              |
| 1:6:1586:A:H2'     | 1:6:1587:A:O4'     | 2.18                     | 0.42              |
| 2:s0:139:VAL:HG22  | 4:s2:62:PRO:HG3    | 2.01                     | 0.42              |
| 2:s0:200:ASP:OD2   | 2:s0:203:PHE:HE1   | 2.02                     | 0.42              |
| 4:s2:125:ILE:O     | 4:s2:129:ILE:HG13  | 2.19                     | 0.42              |
| 10:s8:42:ARG:HB3   | 10:s8:59:ARG:HB2   | 2.00                     | 0.42              |
| 11:s9:3:ARG:HD3    | 11:s9:3:ARG:H      | 1.84                     | 0.42              |
| 14:c2:58:LEU:HA    | 14:c2:87:PRO:HG3   | 2.01                     | 0.42              |
| 17:c5:79:HIS:O     | 17:c5:81:ARG:N     | 2.52                     | 0.42              |
| 21:c9:45:MET:HE3   | 21:c9:45:MET:HB3   | 1.78                     | 0.42              |
| 24:d2:67:GLY:C     | 24:d2:69:LEU:H     | 2.27                     | 0.42              |
| 80:e0:36:LYS:HD3   | 80:e0:36:LYS:HA    | 1.68                     | 0.42              |
| 33:e1:77:GLY:HA2   | 33:e1:78:LYS:HA    | 1.70                     | 0.42              |
| 36:5:59:G:H4'      | 36:5:60:A:H4'      | 2.00                     | 0.42              |
| 36:5:1340:G:H2'    | 36:5:1341:U:H6     | 1.84                     | 0.42              |
| 36:5:1814:A:OP1    | 86:5:4178:OHX:N3   | 2.52                     | 0.42              |
| 36:5:3087:A:H2'    | 36:5:3088:G:O4'    | 2.19                     | 0.42              |
| 36:5:3174:A:N6     | 36:5:3278:C:C2     | 2.87                     | 0.42              |
| 86:5:4033:OHX:N1   | 86:5:4081:OHX:N2   | 2.66                     | 0.42              |
| 41:l4:262:TRP:O    | 41:l4:276:LEU:HD11 | 2.19                     | 0.42              |
| 42:l5:68:THR:HB    | 42:l5:71:GLY:O     | 2.19                     | 0.42              |
| 46:l9:113:GLU:HA   | 46:l9:124:ARG:O    | 2.19                     | 0.42              |
| 52:m6:138:LEU:HD12 | 52:m6:138:LEU:HA   | 1.70                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2:131:C:O2'      | 1:2:132:U:OP1     | 2.33                     | 0.42              |
| 1:2:622:A:H4'      | 1:2:623:A:OP1     | 2.19                     | 0.42              |
| 1:2:1313:A:H2'     | 1:2:1315:U:H5'    | 2.00                     | 0.42              |
| 86:2:2167:OHX:N1   | 86:2:2168:OHX:N3  | 2.67                     | 0.42              |
| 13:C1:97:TYR:O     | 13:C1:99:ARG:HG2  | 2.19                     | 0.42              |
| 18:C6:45:ARG:O     | 18:C6:48:VAL:HG12 | 2.19                     | 0.42              |
| 30:D8:50:GLU:O     | 30:D8:51:ASN:HB2  | 2.19                     | 0.42              |
| 34:SR:4:ASN:HA     | 34:SR:318:ALA:HB2 | 2.01                     | 0.42              |
| 36:1:146:U:H5''    | 36:1:148:G:O4'    | 2.18                     | 0.42              |
| 36:1:637:C:H2'     | 36:1:638:C:H6     | 1.81                     | 0.42              |
| 36:1:1631:C:OP2    | 63:N7:48:ARG:NH2  | 2.48                     | 0.42              |
| 36:1:1719:G:OP1    | 55:M9:110:ARG:NH2 | 2.53                     | 0.42              |
| 36:1:1908:A:H8     | 36:1:1908:A:O5'   | 2.00                     | 0.42              |
| 36:1:2873:U:H5     | 36:1:2941:A:H2    | 1.67                     | 0.42              |
| 36:1:3033:A:H2'    | 36:1:3034:C:H6    | 1.83                     | 0.42              |
| 38:4:52:A:H62      | 75:O9:27:ILE:CD1  | 2.30                     | 0.42              |
| 40:L3:19:ARG:HG3   | 40:L3:273:HIS:NE2 | 2.34                     | 0.42              |
| 43:L6:55:LEU:HD23  | 43:L6:55:LEU:HA   | 1.88                     | 0.42              |
| 43:L6:98:VAL:HA    | 43:L6:101:PHE:HD2 | 1.84                     | 0.42              |
| 45:L8:109:LEU:O    | 45:L8:113:ALA:N   | 2.36                     | 0.42              |
| 48:M1:60:ARG:HH11  | 48:M1:60:ARG:HB2  | 1.84                     | 0.42              |
| 55:M9:104:ARG:HH22 | 55:M9:135:LYS:HD2 | 1.84                     | 0.42              |
| 59:N3:4:ASN:C      | 59:N3:6:ALA:H     | 2.26                     | 0.42              |
| 64:N8:96:LYS:HB3   | 64:N8:97:GLU:H    | 1.75                     | 0.42              |
| 72:O6:97:SER:O     | 72:O6:99:ARG:N    | 2.52                     | 0.42              |
| 74:O8:41:THR:HG21  | 74:O8:62:ALA:CB   | 2.49                     | 0.42              |
| 1:6:1:U:H1'        | 1:6:369:A:C8      | 2.55                     | 0.42              |
| 1:6:5:U:H2'        | 1:6:6:G:H8        | 1.83                     | 0.42              |
| 1:6:192:U:H1'      | 1:6:193:U:C4      | 2.54                     | 0.42              |
| 1:6:1254:U:OP1     | 33:e1:143:LYS:HD3 | 2.19                     | 0.42              |
| 3:s1:116:LYS:HE2   | 3:s1:117:TRP:CZ2  | 2.54                     | 0.42              |
| 5:s3:132:LYS:HB3   | 5:s3:189:MET:HG3  | 2.00                     | 0.42              |
| 5:s3:167:PHE:O     | 5:s3:190:ARG:HG2  | 2.19                     | 0.42              |
| 6:s4:124:GLY:HA2   | 6:s4:142:HIS:CE1  | 2.55                     | 0.42              |
| 9:s7:158:ASP:C     | 9:s7:160:GLN:N    | 2.77                     | 0.42              |
| 10:s8:115:ALA:O    | 10:s8:116:HIS:C   | 2.63                     | 0.42              |
| 18:c6:97:VAL:HG12  | 18:c6:98:ASP:H    | 1.85                     | 0.42              |
| 19:c7:13:SER:HA    | 19:c7:54:THR:HG22 | 2.01                     | 0.42              |
| 23:d1:38:LYS:HE3   | 23:d1:38:LYS:HB2  | 1.72                     | 0.42              |
| 29:d7:62:ILE:HA    | 29:d7:62:ILE:HD12 | 1.79                     | 0.42              |
| 36:5:76:G:O6       | 49:m3:101:ARG:HA  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:109:A:H4'     | 36:5:110:G:H5'     | 2.00                     | 0.42              |
| 36:5:111:C:O2'     | 36:5:112:U:H5'     | 2.19                     | 0.42              |
| 36:5:121:A:C4      | 45:l8:108:ARG:NH1  | 2.87                     | 0.42              |
| 36:5:192:C:H2'     | 36:5:193:C:C6      | 2.55                     | 0.42              |
| 36:5:900:G:H1'     | 36:5:1589:A:H61    | 1.84                     | 0.42              |
| 36:5:1151:U:H3'    | 36:5:1152:G:C8     | 2.54                     | 0.42              |
| 36:5:1801:U:H2'    | 36:5:1802:C:C6     | 2.55                     | 0.42              |
| 36:5:2939:G:OP2    | 40:l3:3:HIS:HD2    | 2.01                     | 0.42              |
| 36:5:3309:G:H1'    | 53:m7:69:ARG:HD3   | 2.00                     | 0.42              |
| 86:5:4033:OHX:N3   | 86:5:4081:OHX:N4   | 2.67                     | 0.42              |
| 38:8:38:U:C5       | 71:o5:82:ALA:O     | 2.72                     | 0.42              |
| 39:l2:61:VAL:HG22  | 39:l2:63:PHE:CE1   | 2.54                     | 0.42              |
| 40:l3:4:ARG:HG3    | 40:l3:4:ARG:NH1    | 2.34                     | 0.42              |
| 41:l4:10:SER:OG    | 41:l4:14:GLU:HG3   | 2.19                     | 0.42              |
| 41:l4:89:ALA:O     | 41:l4:90:PHE:O     | 2.38                     | 0.42              |
| 53:m7:26:PHE:HE1   | 53:m7:120:ASN:HA   | 1.84                     | 0.42              |
| 54:m8:94:PHE:CZ    | 64:n8:119:PRO:HD3  | 2.54                     | 0.42              |
| 61:n5:121:LYS:HD2  | 61:n5:123:TYR:CZ   | 2.54                     | 0.42              |
| 63:n7:46:ILE:HD13  | 63:n7:49:TYR:HA    | 2.01                     | 0.42              |
| 1:2:702:G:C2       | 1:2:703:G:H1'      | 2.55                     | 0.42              |
| 1:2:901:G:H22      | 16:C4:54:GLU:CD    | 2.27                     | 0.42              |
| 1:2:1165:G:C6      | 1:2:1166:A:C6      | 3.07                     | 0.42              |
| 2:S0:105:GLY:O     | 2:S0:112:THR:HG21  | 2.18                     | 0.42              |
| 6:S4:121:TYR:HA    | 6:S4:163:ASP:O     | 2.19                     | 0.42              |
| 7:S5:99:MET:HG3    | 7:S5:180:ARG:NH2   | 2.34                     | 0.42              |
| 11:S9:11:THR:O     | 11:S9:44:ARG:HG3   | 2.18                     | 0.42              |
| 11:S9:171:ARG:O    | 11:S9:175:ARG:HB2  | 2.19                     | 0.42              |
| 13:C1:57:LYS:HB2   | 13:C1:110:HIS:CE1  | 2.54                     | 0.42              |
| 14:C2:40:GLY:O     | 14:C2:124:LYS:N    | 2.51                     | 0.42              |
| 22:D0:96:PRO:HG2   | 22:D0:99:ILE:HG22  | 2.01                     | 0.42              |
| 24:D2:105:THR:HG23 | 24:D2:110:ILE:HG12 | 2.02                     | 0.42              |
| 27:D5:70:LYS:HB3   | 27:D5:71:ILE:HG13  | 2.01                     | 0.42              |
| 36:1:1073:U:O2'    | 65:N9:49:GLY:HA3   | 2.19                     | 0.42              |
| 36:1:1815:U:H1'    | 36:1:1816:A:O5'    | 2.19                     | 0.42              |
| 36:1:2565:U:H2'    | 36:1:2566:C:C6     | 2.54                     | 0.42              |
| 36:1:2796:G:N7     | 78:Q2:63:LYS:NZ    | 2.67                     | 0.42              |
| 36:1:2970:C:H4'    | 36:1:2971:A:C2     | 2.54                     | 0.42              |
| 36:1:3106:A:H2'    | 36:1:3107:U:O4'    | 2.19                     | 0.42              |
| 36:1:3123:A:O2'    | 46:L9:40:HIS:ND1   | 2.50                     | 0.42              |
| 37:3:28:C:OP1      | 48:M1:137:ARG:HD3  | 2.19                     | 0.42              |
| 38:4:24:G:OP2      | 62:N6:13:ARG:HD3   | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:L4:62:ALA:HB2   | 41:L4:77:VAL:HA    | 2.02                     | 0.42              |
| 44:L7:211:SER:O    | 44:L7:213:GLY:N    | 2.51                     | 0.42              |
| 46:L9:4:ILE:CD1    | 56:N0:148:LEU:HD11 | 2.49                     | 0.42              |
| 54:M8:11:LYS:HB3   | 54:M8:11:LYS:HE3   | 1.84                     | 0.42              |
| 57:N1:14:MET:HE2   | 57:N1:15:PHE:CE2   | 2.55                     | 0.42              |
| 61:N5:132:ALA:HA   | 61:N5:135:ILE:HG22 | 2.02                     | 0.42              |
| 63:N7:77:TYR:C     | 63:N7:79:HIS:H     | 2.28                     | 0.42              |
| 64:N8:133:LEU:HD13 | 64:N8:137:LYS:HE3  | 2.01                     | 0.42              |
| 1:6:1039:A:H5''    | 23:d1:62:ARG:NH2   | 2.35                     | 0.42              |
| 2:s0:175:TYR:OH    | 2:s0:195:TRP:HB3   | 2.18                     | 0.42              |
| 3:s1:117:TRP:O     | 3:s1:153:HIS:O     | 2.37                     | 0.42              |
| 6:s4:65:LEU:HD23   | 6:s4:70:VAL:HG13   | 2.01                     | 0.42              |
| 9:s7:44:LYS:HG3    | 9:s7:63:PRO:HD3    | 2.01                     | 0.42              |
| 11:s9:3:ARG:HD3    | 11:s9:3:ARG:N      | 2.34                     | 0.42              |
| 13:c1:80:MET:HE2   | 13:c1:80:MET:HB2   | 1.67                     | 0.42              |
| 20:c8:4:VAL:HG21   | 27:d5:82:HIS:CG    | 2.55                     | 0.42              |
| 21:c9:57:ARG:HG3   | 21:c9:57:ARG:NH1   | 2.18                     | 0.42              |
| 24:d2:89:TRP:HE3   | 24:d2:93:LEU:HD22  | 1.84                     | 0.42              |
| 36:5:80:G:H2'      | 36:5:81:C:C6       | 2.54                     | 0.42              |
| 36:5:422:A:C2      | 36:5:2363:A:H4'    | 2.55                     | 0.42              |
| 36:5:959:C:OP2     | 36:5:960:U:C5      | 2.73                     | 0.42              |
| 36:5:1252:A:H2     | 36:5:1263:A:C2     | 2.38                     | 0.42              |
| 36:5:1588:A:C6     | 75:o9:4:GLN:HG2    | 2.55                     | 0.42              |
| 36:5:2512:C:N4     | 36:5:2513:U:O4     | 2.53                     | 0.42              |
| 36:5:2653:C:OP1    | 78:q2:89:LYS:HB2   | 2.20                     | 0.42              |
| 36:5:2881:C:H2'    | 36:5:2882:U:C6     | 2.55                     | 0.42              |
| 41:l4:182:LEU:HD13 | 41:l4:182:LEU:HA   | 1.69                     | 0.42              |
| 42:l5:257:GLU:CD   | 42:l5:257:GLU:N    | 2.78                     | 0.42              |
| 43:l6:60:ASP:O     | 43:l6:61:ASN:HB2   | 2.20                     | 0.42              |
| 43:l6:82:ARG:NH1   | 69:o3:106:ASN:HB2  | 2.34                     | 0.42              |
| 46:l9:92:TYR:HD2   | 46:l9:179:ILE:HG23 | 1.83                     | 0.42              |
| 48:m1:93:ASP:C     | 48:m1:94:ARG:O     | 2.62                     | 0.42              |
| 49:m3:67:ARG:H     | 49:m3:67:ARG:HG3   | 1.46                     | 0.42              |
| 53:m7:136:ILE:HG23 | 53:m7:136:ILE:HD12 | 1.80                     | 0.42              |
| 61:n5:23:ALA:O     | 61:n5:24:LEU:HB2   | 2.19                     | 0.42              |
| 66:o0:17:VAL:HG21  | 66:o0:100:ILE:HD13 | 2.02                     | 0.42              |
| 67:o1:80:ASN:OD1   | 67:o1:81:GLU:N     | 2.52                     | 0.42              |
| 72:o6:4:LYS:HD2    | 72:o6:14:GLY:HA3   | 2.02                     | 0.42              |
| 1:2:545:A:H4'      | 1:2:546:U:OP1      | 2.20                     | 0.42              |
| 1:2:603:U:H2'      | 1:2:604:A:C8       | 2.54                     | 0.42              |
| 1:2:694:U:H5       | 9:S7:96:ARG:O      | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:809:A:C6      | 1:2:810:G:C6       | 3.07                     | 0.42              |
| 1:2:872:G:H2'     | 1:2:873:U:O4'      | 2.20                     | 0.42              |
| 1:2:964:U:OP1     | 15:C3:128:TYR:OH   | 2.31                     | 0.42              |
| 1:2:972:G:O2'     | 36:1:847:A:N1      | 2.49                     | 0.42              |
| 1:2:1519:U:H2'    | 1:2:1520:U:C5      | 2.54                     | 0.42              |
| 1:2:1756:A:OP2    | 1:2:1756:A:H8      | 2.02                     | 0.42              |
| 3:S1:61:LEU:HD22  | 3:S1:61:LEU:H      | 1.83                     | 0.42              |
| 4:S2:86:VAL:C     | 4:S2:87:GLN:HG2    | 2.45                     | 0.42              |
| 6:S4:193:GLY:O    | 6:S4:210:ILE:HG23  | 2.19                     | 0.42              |
| 8:S6:119:GLN:HG3  | 8:S6:120:GLU:N     | 2.35                     | 0.42              |
| 9:S7:111:LYS:O    | 9:S7:112:ARG:HB2   | 2.19                     | 0.42              |
| 10:S8:57:ALA:HB2  | 10:S8:177:GLY:HA2  | 2.01                     | 0.42              |
| 35:SM:116:GLU:O   | 35:SM:119:ALA:N    | 2.47                     | 0.42              |
| 36:1:126:U:OP1    | 51:M5:144:ARG:NH1  | 2.47                     | 0.42              |
| 36:1:601:U:H2'    | 36:1:602:A:O4'     | 2.18                     | 0.42              |
| 36:1:638:C:H2'    | 36:1:639:G:C8      | 2.54                     | 0.42              |
| 36:1:908:G:H4'    | 36:1:909:G:O5'     | 2.19                     | 0.42              |
| 36:1:1073:U:H1'   | 65:N9:50:THR:HG22  | 2.00                     | 0.42              |
| 36:1:1162:U:H4'   | 68:O2:57:TYR:CE1   | 2.55                     | 0.42              |
| 36:1:1373:A:H2'   | 36:1:1374:G:C8     | 2.55                     | 0.42              |
| 36:1:1485:G:N2    | 70:O4:4:ARG:HD2    | 2.34                     | 0.42              |
| 36:1:1668:G:C6    | 36:1:1669:C:C4     | 3.08                     | 0.42              |
| 36:1:2686:A:OP2   | 86:1:3903:OHX:N2   | 2.52                     | 0.42              |
| 36:1:2878:G:H5''  | 40:L3:5:LYS:HE2    | 2.00                     | 0.42              |
| 36:1:3193:C:H2'   | 36:1:3194:C:O4'    | 2.20                     | 0.42              |
| 38:4:41:A:O2'     | 73:O7:59:THR:HB    | 2.18                     | 0.42              |
| 40:L3:43:LEU:HD22 | 40:L3:203:VAL:HG11 | 2.02                     | 0.42              |
| 40:L3:114:VAL:O   | 40:L3:117:ARG:HB3  | 2.20                     | 0.42              |
| 41:L4:285:ASP:OD2 | 41:L4:288:ARG:HB2  | 2.19                     | 0.42              |
| 42:L5:21:ARG:HA   | 42:L5:24:ARG:NH2   | 2.35                     | 0.42              |
| 42:L5:34:LYS:HE3  | 57:N1:30:TYR:OH    | 2.19                     | 0.42              |
| 51:M5:184:LYS:C   | 51:M5:186:GLY:H    | 2.25                     | 0.42              |
| 54:M8:178:ARG:HD3 | 54:M8:178:ARG:HA   | 1.80                     | 0.42              |
| 55:M9:10:LEU:HD12 | 55:M9:10:LEU:HA    | 1.82                     | 0.42              |
| 1:6:272:U:O3'     | 60:n4:123:ARG:HD3  | 2.20                     | 0.42              |
| 1:6:312:A:C2      | 1:6:314:C:H2'      | 2.54                     | 0.42              |
| 1:6:602:U:H2'     | 1:6:603:U:C6       | 2.54                     | 0.42              |
| 1:6:1082:C:H2'    | 1:6:1083:G:O4'     | 2.20                     | 0.42              |
| 1:6:1211:A:H1'    | 17:c5:99:GLY:O     | 2.19                     | 0.42              |
| 1:6:1638:G:C2     | 1:6:1639:C:H1'     | 2.54                     | 0.42              |
| 86:6:2121:OHX:N4  | 86:6:2171:OHX:N1   | 2.67                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:s0:22:THR:HG22   | 2:s0:169:SER:OG    | 2.19                     | 0.42              |
| 3:s1:144:ARG:HB3   | 3:s1:208:GLN:HG2   | 2.00                     | 0.42              |
| 3:s1:223:PHE:O     | 3:s1:224:ASP:HB3   | 2.20                     | 0.42              |
| 6:s4:104:ASP:HB3   | 6:s4:106:LYS:H     | 1.85                     | 0.42              |
| 7:s5:44:ASN:H      | 7:s5:44:ASN:HD22   | 1.68                     | 0.42              |
| 9:s7:126:LEU:HD13  | 9:s7:173:TYR:CD2   | 2.54                     | 0.42              |
| 9:s7:166:LEU:HA    | 9:s7:166:LEU:HD12  | 1.71                     | 0.42              |
| 10:s8:10:LYS:HG2   | 13:c1:133:LYS:CE   | 2.49                     | 0.42              |
| 26:d4:52:LYS:O     | 26:d4:54:ALA:N     | 2.53                     | 0.42              |
| 28:d6:8:ASN:HB2    | 28:d6:9:GLY:H      | 1.50                     | 0.42              |
| 31:d9:26:SER:OG    | 31:d9:27:HIS:N     | 2.52                     | 0.42              |
| 34:sR:106:HIS:ND1  | 34:sR:128:ASP:OD2  | 2.43                     | 0.42              |
| 36:5:123:A:C6      | 36:5:150:A:C5      | 3.08                     | 0.42              |
| 36:5:284:A:H4'     | 36:5:285:A:C2      | 2.55                     | 0.42              |
| 36:5:1070:U:C4     | 36:5:1071:U:C4     | 3.07                     | 0.42              |
| 36:5:1500:G:H2'    | 36:5:1501:U:H6     | 1.84                     | 0.42              |
| 36:5:2390:A:H2'    | 36:5:2391:G:O4'    | 2.20                     | 0.42              |
| 36:5:2586:G:C5     | 45:l8:241:LYS:HB2  | 2.54                     | 0.42              |
| 37:7:6:C:O2'       | 42:l5:72:ASP:OD2   | 2.35                     | 0.42              |
| 38:8:4:C:H2'       | 38:8:5:U:H6        | 1.83                     | 0.42              |
| 41:l4:52:VAL:HG21  | 41:l4:99:MET:HE2   | 2.02                     | 0.42              |
| 41:l4:91:GLY:O     | 41:l4:94:CYS:HB2   | 2.19                     | 0.42              |
| 42:l5:146:LEU:HD13 | 42:l5:148:ILE:HD11 | 2.02                     | 0.42              |
| 44:l7:128:LYS:C    | 44:l7:130:ILE:H    | 2.27                     | 0.42              |
| 44:l7:158:LYS:C    | 44:l7:158:LYS:CD   | 2.93                     | 0.42              |
| 47:m0:88:ARG:HG2   | 47:m0:90:ARG:HG2   | 2.02                     | 0.42              |
| 59:n3:13:ILE:HD12  | 59:n3:85:TRP:CG    | 2.54                     | 0.42              |
| 63:n7:83:THR:HG23  | 63:n7:85:TYR:H     | 1.83                     | 0.42              |
| 74:o8:3:ARG:NH1    | 74:o8:52:TYR:HE1   | 2.17                     | 0.42              |
| 75:o9:48:LYS:HD2   | 75:o9:48:LYS:HA    | 1.74                     | 0.42              |
| 82:p0:29:GLY:HA2   | 82:p0:84:VAL:HG12  | 2.02                     | 0.42              |
| 1:2:149:C:H2'      | 1:2:150:U:C6       | 2.55                     | 0.42              |
| 1:2:538:A:C8       | 1:2:543:C:C4       | 3.07                     | 0.42              |
| 1:2:707:A:O2'      | 1:2:731:C:N4       | 2.53                     | 0.42              |
| 1:2:1511:U:H2'     | 1:2:1512:G:H8      | 1.85                     | 0.42              |
| 2:S0:126:PRO:HB2   | 2:S0:152:PRO:HG2   | 2.01                     | 0.42              |
| 3:S1:115:ARG:HG3   | 3:S1:116:LYS:N     | 2.34                     | 0.42              |
| 5:S3:29:LEU:HB2    | 5:S3:34:TYR:HB2    | 2.01                     | 0.42              |
| 7:S5:112:ARG:NH1   | 18:C6:43:ILE:HD11  | 2.33                     | 0.42              |
| 11:S9:149:ARG:H    | 11:S9:149:ARG:HD3  | 1.85                     | 0.42              |
| 13:C1:29:LYS:O     | 13:C1:31:THR:N     | 2.46                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:C8:94:ASP:CG   | 20:C8:96:LYS:HG3   | 2.45                     | 0.42              |
| 22:D0:57:ARG:HD2  | 22:D0:89:ARG:HD3   | 2.02                     | 0.42              |
| 24:D2:122:SER:OG  | 24:D2:123:GLY:N    | 2.53                     | 0.42              |
| 26:D4:27:VAL:HG21 | 26:D4:40:LEU:HD11  | 2.01                     | 0.42              |
| 26:D4:62:THR:HB   | 26:D4:69:SER:OG    | 2.19                     | 0.42              |
| 36:1:437:G:H2'    | 36:1:438:A:O4'     | 2.19                     | 0.42              |
| 36:1:612:U:H2'    | 36:1:613:G:H8      | 1.84                     | 0.42              |
| 36:1:1074:U:O2'   | 36:1:1075:A:H2'    | 2.19                     | 0.42              |
| 37:3:28:C:H1'     | 37:3:55:A:H61      | 1.83                     | 0.42              |
| 37:3:64:A:H3'     | 47:M0:204:GLY:O    | 2.18                     | 0.42              |
| 42:L5:188:GLU:O   | 42:L5:188:GLU:HG3  | 2.20                     | 0.42              |
| 42:L5:196:ARG:HB3 | 42:L5:196:ARG:HH11 | 1.85                     | 0.42              |
| 44:L7:25:GLN:O    | 44:L7:26:VAL:C     | 2.63                     | 0.42              |
| 45:L8:72:PRO:HA   | 45:L8:73:PRO:HD3   | 1.87                     | 0.42              |
| 46:L9:124:ARG:HD3 | 46:L9:164:ILE:O    | 2.19                     | 0.42              |
| 47:M0:63:GLU:HG2  | 47:M0:63:GLU:H     | 1.35                     | 0.42              |
| 58:N2:17:VAL:HA   | 58:N2:103:TYR:O    | 2.20                     | 0.42              |
| 58:N2:35:LYS:O    | 58:N2:38:ILE:HB    | 2.19                     | 0.42              |
| 58:N2:99:LYS:HE3  | 58:N2:102:GLU:HB2  | 2.01                     | 0.42              |
| 59:N3:90:GLY:O    | 60:N4:16:GLY:HA2   | 2.19                     | 0.42              |
| 60:N4:55:PHE:CE2  | 60:N4:59:HIS:CE1   | 3.07                     | 0.42              |
| 1:6:187:G:H8      | 1:6:187:G:O5'      | 2.01                     | 0.42              |
| 1:6:704:C:H2'     | 1:6:705:U:O4'      | 2.20                     | 0.42              |
| 1:6:902:G:H2'     | 1:6:903:U:C6       | 2.54                     | 0.42              |
| 1:6:926:A:H1'     | 1:6:988:A:C2       | 2.55                     | 0.42              |
| 1:6:1253:U:H2'    | 1:6:1254:U:O4'     | 2.19                     | 0.42              |
| 1:6:1388:A:H4'    | 1:6:1389:C:O5'     | 2.20                     | 0.42              |
| 1:6:1752:U:H2'    | 1:6:1753:A:C8      | 2.54                     | 0.42              |
| 3:s1:106:THR:HA   | 16:c4:116:GLU:OE1  | 2.18                     | 0.42              |
| 3:s1:206:PRO:O    | 3:s1:207:LEU:HB2   | 2.20                     | 0.42              |
| 4:s2:115:ILE:HD13 | 4:s2:208:GLU:OE1   | 2.20                     | 0.42              |
| 6:s4:181:VAL:HG21 | 6:s4:195:ILE:HD11  | 2.01                     | 0.42              |
| 8:s6:151:ASP:OD2  | 60:n4:101:ARG:HD3  | 2.18                     | 0.42              |
| 14:c2:83:GLU:C    | 14:c2:85:LYS:H     | 2.28                     | 0.42              |
| 17:c5:74:ALA:HA   | 17:c5:75:PRO:HD3   | 1.91                     | 0.42              |
| 25:d3:23:ARG:HD3  | 25:d3:26:GLU:OE1   | 2.20                     | 0.42              |
| 36:5:702:C:O2     | 36:5:788:C:H4'     | 2.20                     | 0.42              |
| 36:5:1491:A:H5'   | 73:o7:12:HIS:O     | 2.20                     | 0.42              |
| 36:5:1613:A:OP1   | 74:o8:2:ALA:HB3    | 2.19                     | 0.42              |
| 36:5:1786:G:H2'   | 36:5:1787:A:C8     | 2.54                     | 0.42              |
| 36:5:2737:C:H4'   | 57:n1:68:THR:OG1   | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:5:4023:OHX:N2   | 86:5:4215:OHX:N5   | 2.67                     | 0.42              |
| 86:5:4076:OHX:N3   | 86:o4:203:OHX:N6   | 2.67                     | 0.42              |
| 42:l5:224:LYS:HE3  | 42:l5:224:LYS:HB2  | 1.78                     | 0.42              |
| 45:l8:189:LEU:O    | 45:l8:190:VAL:HG23 | 2.20                     | 0.42              |
| 46:l9:95:ALA:HA    | 76:q0:78:ILE:HG22  | 2.00                     | 0.42              |
| 48:m1:131:MET:HE3  | 48:m1:131:MET:HB3  | 1.79                     | 0.42              |
| 49:m3:70:ARG:HD2   | 49:m3:71:ALA:O     | 2.19                     | 0.42              |
| 52:m6:38:ALA:O     | 52:m6:41:LEU:HB2   | 2.20                     | 0.42              |
| 56:n0:139:TYR:CD2  | 56:n0:140:VAL:HG23 | 2.54                     | 0.42              |
| 72:o6:57:LEU:HB2   | 72:o6:90:MET:HE3   | 2.02                     | 0.42              |
| 1:2:51:A:OP2       | 86:2:2073:OHX:N3   | 2.53                     | 0.42              |
| 1:2:74:U:O2'       | 1:2:75:U:OP2       | 2.36                     | 0.42              |
| 1:2:558:U:HO2'     | 1:2:559:C:P        | 2.42                     | 0.42              |
| 1:2:624:G:OP2      | 86:2:2158:OHX:N2   | 2.53                     | 0.42              |
| 1:2:814:A:OP1      | 55:M9:170:ARG:NH2  | 2.48                     | 0.42              |
| 1:2:978:A:H2'      | 1:2:979:A:O4'      | 2.20                     | 0.42              |
| 1:2:1317:C:H2'     | 1:2:1318:G:O4'     | 2.20                     | 0.42              |
| 1:2:1480:G:H3'     | 1:2:1481:C:C6      | 2.55                     | 0.42              |
| 2:S0:52:LYS:H      | 2:S0:52:LYS:HG2    | 1.35                     | 0.42              |
| 3:S1:67:GLU:OE2    | 3:S1:83:LYS:HE3    | 2.19                     | 0.42              |
| 6:S4:95:THR:O      | 6:S4:97:GLU:HG3    | 2.20                     | 0.42              |
| 6:S4:127:LYS:HG3   | 6:S4:142:HIS:HA    | 2.02                     | 0.42              |
| 9:S7:35:LYS:HG2    | 9:S7:36:ALA:H      | 1.84                     | 0.42              |
| 25:D3:59:ILE:CD1   | 32:E0:4:VAL:HG13   | 2.49                     | 0.42              |
| 34:SR:49:GLY:O     | 34:SR:51:ASP:N     | 2.44                     | 0.42              |
| 34:SR:112:SER:HB2  | 34:SR:153:GLN:HA   | 2.01                     | 0.42              |
| 34:SR:117:LYS:HE2  | 34:SR:117:LYS:H    | 1.84                     | 0.42              |
| 36:1:907:G:O2'     | 36:1:926:A:N7      | 2.47                     | 0.42              |
| 36:1:916:G:N1      | 39:L2:207:VAL:HG11 | 2.35                     | 0.42              |
| 36:1:1081:U:H6     | 36:1:1081:U:H2'    | 1.58                     | 0.42              |
| 36:1:1638:A:N3     | 36:1:1709:C:H1'    | 2.34                     | 0.42              |
| 36:1:2414:G:H2'    | 36:1:2415:C:O4'    | 2.19                     | 0.42              |
| 36:1:2988:C:O2     | 40:L3:266:ARG:NH1  | 2.52                     | 0.42              |
| 36:1:3174:A:H2'    | 36:1:3175:U:H5'    | 2.01                     | 0.42              |
| 40:L3:211:GLN:NE2  | 40:L3:284:ARG:HA   | 2.34                     | 0.42              |
| 40:L3:244:ARG:HG2  | 40:L3:244:ARG:HH11 | 1.84                     | 0.42              |
| 42:L5:148:ILE:HD13 | 42:L5:148:ILE:HG21 | 1.73                     | 0.42              |
| 43:L6:173:MET:HE3  | 43:L6:173:MET:HB3  | 1.60                     | 0.42              |
| 45:L8:50:VAL:HG11  | 61:N5:27:ARG:HG3   | 2.00                     | 0.42              |
| 49:M3:174:ARG:CZ   | 72:O6:9:ILE:HD13   | 2.50                     | 0.42              |
| 50:M4:53:VAL:HA    | 50:M4:54:PRO:HD3   | 1.82                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:M5:135:VAL:CG1 | 51:M5:142:ILE:HG12 | 2.50                     | 0.42              |
| 52:M6:39:GLU:HG2  | 52:M6:40:GLU:HG2   | 2.01                     | 0.42              |
| 54:M8:120:GLU:CD  | 54:M8:122:ILE:HD11 | 2.44                     | 0.42              |
| 61:N5:77:GLU:HG3  | 61:N5:133:LEU:HG   | 2.02                     | 0.42              |
| 65:N9:9:ALA:O     | 65:N9:10:HIS:C     | 2.59                     | 0.42              |
| 68:O2:11:LYS:O    | 68:O2:12:LYS:HB2   | 2.19                     | 0.42              |
| 69:O3:103:TYR:HA  | 69:O3:104:PRO:C    | 2.45                     | 0.42              |
| 1:6:252:U:H4'     | 6:s4:132:GLY:O     | 2.19                     | 0.42              |
| 1:6:871:G:H2'     | 1:6:872:G:C8       | 2.55                     | 0.42              |
| 1:6:874:C:OP1     | 3:s1:159:SER:OG    | 2.31                     | 0.42              |
| 1:6:1382:A:H5''   | 22:d0:60:THR:HG22  | 2.02                     | 0.42              |
| 1:6:1471:A:OP1    | 7:s5:185:ARG:NH1   | 2.53                     | 0.42              |
| 1:6:1590:G:H2'    | 1:6:1591:C:H6      | 1.85                     | 0.42              |
| 2:s0:180:GLU:OE2  | 2:s0:191:ARG:NH2   | 2.52                     | 0.42              |
| 5:s3:215:GLU:HA   | 5:s3:216:PRO:HD2   | 1.92                     | 0.42              |
| 6:s4:163:ASP:HB3  | 6:s4:167:GLY:O     | 2.20                     | 0.42              |
| 6:s4:248:ILE:HG13 | 11:s9:71:PHE:CD2   | 2.55                     | 0.42              |
| 14:c2:62:LEU:HB3  | 14:c2:120:VAL:HG13 | 2.02                     | 0.42              |
| 15:c3:64:ARG:HG3  | 15:c3:70:LYS:HD2   | 2.02                     | 0.42              |
| 15:c3:65:VAL:HG23 | 15:c3:66:ILE:CG2   | 2.47                     | 0.42              |
| 33:e1:121:CYS:HB2 | 33:e1:132:LEU:HD21 | 2.02                     | 0.42              |
| 36:5:177:U:OP2    | 86:5:4017:OHX:N6   | 2.52                     | 0.42              |
| 36:5:315:C:OP2    | 72:o6:28:TYR:OH    | 2.35                     | 0.42              |
| 36:5:685:G:P      | 49:m3:35:ARG:NH1   | 2.92                     | 0.42              |
| 36:5:1817:G:O2'   | 36:5:1818:U:OP2    | 2.32                     | 0.42              |
| 36:5:2611:U:H2'   | 36:5:2612:U:C6     | 2.55                     | 0.42              |
| 86:5:4034:OHX:N1  | 86:5:4117:OHX:N3   | 2.68                     | 0.42              |
| 38:8:62:C:H4'     | 38:8:63:G:O5'      | 2.20                     | 0.42              |
| 39:l2:205:ASN:O   | 39:l2:206:PRO:C    | 2.62                     | 0.42              |
| 43:l6:2:SER:HA    | 68:o2:81:ASP:CG    | 2.45                     | 0.42              |
| 47:m0:45:GLU:O    | 47:m0:141:LYS:HE3  | 2.19                     | 0.42              |
| 51:m5:174:ILE:O   | 51:m5:174:ILE:HG22 | 2.19                     | 0.42              |
| 54:m8:19:PRO:HD3  | 54:m8:30:VAL:HG21  | 2.01                     | 0.42              |
| 54:m8:182:LYS:HA  | 54:m8:182:LYS:HD3  | 1.90                     | 0.42              |
| 57:n1:122:GLN:C   | 57:n1:124:VAL:H    | 2.28                     | 0.42              |
| 63:n7:22:LYS:HE3  | 63:n7:134:LEU:HB2  | 2.01                     | 0.42              |
| 1:2:413:U:H2'     | 1:2:414:C:C6       | 2.54                     | 0.42              |
| 1:2:1773:C:OP2    | 77:Q1:2:ARG:HD2    | 2.20                     | 0.42              |
| 5:S3:178:ARG:HE   | 5:S3:178:ARG:N     | 2.16                     | 0.42              |
| 8:S6:63:MET:HA    | 8:S6:98:ARG:O      | 2.20                     | 0.42              |
| 17:C5:48:GLY:O    | 17:C5:52:LYS:HD3   | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:D1:64:GLU:HG3   | 29:D7:3:LEU:HG     | 2.01                     | 0.42              |
| 25:D3:79:ASN:C     | 25:D3:81:LYS:H     | 2.27                     | 0.42              |
| 25:D3:102:VAL:CG1  | 25:D3:127:VAL:HG12 | 2.44                     | 0.42              |
| 26:D4:45:ALA:C     | 26:D4:47:VAL:H     | 2.28                     | 0.42              |
| 34:SR:38:ARG:HG2   | 34:SR:67:ILE:CG2   | 2.49                     | 0.42              |
| 36:1:26:A:C4       | 36:1:330:G:C8      | 3.08                     | 0.42              |
| 36:1:437:G:O2'     | 36:1:438:A:H5'     | 2.20                     | 0.42              |
| 36:1:848:A:H8      | 36:1:848:A:O5'     | 2.03                     | 0.42              |
| 36:1:1069:C:H2'    | 36:1:1070:U:H6     | 1.85                     | 0.42              |
| 36:1:1293:U:O2'    | 36:1:1294:A:H5'    | 2.20                     | 0.42              |
| 36:1:1504:A:C5     | 36:1:1505:C:C5     | 3.08                     | 0.42              |
| 36:1:2186:U:H2'    | 36:1:2187:G:O4'    | 2.19                     | 0.42              |
| 86:1:3955:OHX:N4   | 86:1:4041:OHX:N6   | 2.68                     | 0.42              |
| 41:L4:180:LYS:C    | 41:L4:181:VAL:O    | 2.59                     | 0.42              |
| 42:L5:64:ILE:HD13  | 42:L5:105:ILE:HD12 | 2.01                     | 0.42              |
| 47:M0:76:MET:HE2   | 47:M0:138:VAL:HG11 | 2.02                     | 0.42              |
| 58:N2:79:LEU:O     | 58:N2:82:LYS:HB3   | 2.20                     | 0.42              |
| 64:N8:105:LEU:HB2  | 64:N8:148:ILE:HD11 | 2.01                     | 0.42              |
| 69:O3:89:LEU:HA    | 69:O3:90:PRO:HD3   | 1.76                     | 0.42              |
| 73:O7:69:HIS:ND1   | 73:O7:72:ARG:NH2   | 2.66                     | 0.42              |
| 74:O8:10:GLN:HA    | 74:O8:13:GLU:OE1   | 2.19                     | 0.42              |
| 78:Q2:72:LEU:O     | 78:Q2:80:ARG:HA    | 2.19                     | 0.42              |
| 1:6:93:A:C6        | 1:6:398:G:C6       | 3.08                     | 0.42              |
| 1:6:825:U:O2'      | 1:6:826:U:H6       | 2.02                     | 0.42              |
| 1:6:1175:U:H4'     | 1:6:1196:A:C6      | 2.54                     | 0.42              |
| 1:6:1431:C:H1'     | 1:6:1437:U:O4      | 2.20                     | 0.42              |
| 1:6:1634:C:O2      | 86:6:2156:OHX:N2   | 2.52                     | 0.42              |
| 5:s3:216:PRO:HB2   | 5:s3:217:ILE:H     | 1.53                     | 0.42              |
| 11:s9:110:GLN:HE21 | 11:s9:110:GLN:HA   | 1.84                     | 0.42              |
| 34:sR:307:ASP:O    | 34:sR:308:ASN:HB2  | 2.19                     | 0.42              |
| 36:5:231:G:O6      | 86:5:4132:OHX:N4   | 2.53                     | 0.42              |
| 36:5:1320:C:O2     | 56:n0:115:ARG:NH2  | 2.53                     | 0.42              |
| 36:5:1879:A:H2'    | 36:5:1879:A:N3     | 2.35                     | 0.42              |
| 36:5:2921:U:H2'    | 36:5:2923:U:OP2    | 2.20                     | 0.42              |
| 36:5:2970:C:H4'    | 36:5:2971:A:C2     | 2.55                     | 0.42              |
| 86:5:3973:OHX:N1   | 86:5:4241:OHX:N5   | 2.68                     | 0.42              |
| 38:8:6:U:H2'       | 38:8:7:U:C6        | 2.54                     | 0.42              |
| 38:8:145:U:H2'     | 38:8:146:U:O4'     | 2.20                     | 0.42              |
| 39:l2:36:GLU:OE1   | 39:l2:163:ARG:NH1  | 2.49                     | 0.42              |
| 40:l3:243:HIS:C    | 40:l3:244:ARG:HG3  | 2.45                     | 0.42              |
| 40:l3:258:ALA:O    | 40:l3:259:HIS:CD2  | 2.73                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:l7:229:PHE:C    | 44:l7:229:PHE:HD1  | 2.28                     | 0.42              |
| 45:l8:195:SER:O    | 45:l8:195:SER:OG   | 2.20                     | 0.42              |
| 50:m4:48:GLY:N     | 50:m4:49:PRO:HD3   | 2.35                     | 0.42              |
| 52:m6:73:PHE:CD1   | 52:m6:78:ARG:HG2   | 2.55                     | 0.42              |
| 59:n3:104:ASN:HD21 | 59:n3:108:GLU:HB2  | 1.85                     | 0.42              |
| 62:n6:74:TYR:CZ    | 62:n6:77:LYS:HD2   | 2.54                     | 0.42              |
| 62:n6:103:LYS:HA   | 62:n6:103:LYS:HD3  | 1.71                     | 0.42              |
| 65:n9:32:LEU:O     | 65:n9:33:LYS:C     | 2.63                     | 0.42              |
| 74:o8:8:ILE:HD12   | 74:o8:8:ILE:H      | 1.84                     | 0.42              |
| 75:o9:9:ILE:HG22   | 75:o9:13:MET:HE3   | 2.01                     | 0.42              |
| 76:q0:78:ILE:HG21  | 76:q0:78:ILE:HD13  | 1.75                     | 0.42              |
| 1:2:71:A:N1        | 1:2:72:A:C6        | 2.88                     | 0.42              |
| 1:2:529:A:H2'      | 1:2:530:C:O4'      | 2.20                     | 0.42              |
| 1:2:867:G:OP2      | 15:C3:3:ARG:NH1    | 2.45                     | 0.42              |
| 1:2:927:C:H2'      | 1:2:928:U:C6       | 2.55                     | 0.42              |
| 1:2:1039:A:N6      | 1:2:1091:A:C2      | 2.88                     | 0.42              |
| 1:2:1153:G:H5'     | 28:D6:85:ARG:HD2   | 2.01                     | 0.42              |
| 1:2:1657:U:N3      | 86:2:2090:OHX:N4   | 2.68                     | 0.42              |
| 1:2:1761:U:O2'     | 1:2:1762:A:OP2     | 2.34                     | 0.42              |
| 2:S0:102:PHE:CZ    | 2:S0:106:SER:HB2   | 2.55                     | 0.42              |
| 2:S0:184:LEU:O     | 2:S0:185:ARG:C     | 2.62                     | 0.42              |
| 5:S3:212:LYS:HE2   | 5:S3:212:LYS:HB2   | 1.53                     | 0.42              |
| 7:S5:27:THR:HA     | 7:S5:28:PRO:HD3    | 1.88                     | 0.42              |
| 7:S5:37:GLN:NE2    | 18:C6:46:PHE:CE1   | 2.88                     | 0.42              |
| 9:S7:31:SER:HB2    | 9:S7:32:PRO:HD3    | 2.01                     | 0.42              |
| 12:C0:46:LEU:HD13  | 12:C0:46:LEU:HA    | 1.71                     | 0.42              |
| 15:C3:114:ARG:HA   | 15:C3:114:ARG:HD3  | 1.47                     | 0.42              |
| 16:C4:41:ARG:O     | 16:C4:42:VAL:HG22  | 2.19                     | 0.42              |
| 17:C5:109:PRO:O    | 17:C5:112:LEU:HG   | 2.20                     | 0.42              |
| 18:C6:18:ALA:HB2   | 18:C6:69:VAL:HG13  | 2.01                     | 0.42              |
| 19:C7:84:TYR:C     | 19:C7:85:VAL:HG23  | 2.45                     | 0.42              |
| 21:C9:100:ILE:H    | 21:C9:100:ILE:HG12 | 1.64                     | 0.42              |
| 23:D1:48:GLY:O     | 23:D1:49:GLU:HB2   | 2.18                     | 0.42              |
| 27:D5:93:SER:OG    | 27:D5:100:ILE:N    | 2.53                     | 0.42              |
| 28:D6:6:ALA:C      | 28:D6:8:ASN:H      | 2.28                     | 0.42              |
| 36:1:111:C:O2'     | 36:1:112:U:H5'     | 2.19                     | 0.42              |
| 36:1:191:U:H2'     | 36:1:192:C:H6      | 1.84                     | 0.42              |
| 36:1:1114:U:H5''   | 64:N8:22:ILE:HD12  | 2.02                     | 0.42              |
| 36:1:1686:U:O2     | 36:1:1688:U:H1'    | 2.20                     | 0.42              |
| 36:1:2425:G:H2'    | 36:1:2426:U:O4'    | 2.18                     | 0.42              |
| 36:1:2723:U:H2'    | 36:1:2724:U:C6     | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1:2921:U:H2'    | 36:1:2923:U:H5''   | 2.01                     | 0.42              |
| 36:1:2992:U:H1'    | 53:M7:69:ARG:NH2   | 2.35                     | 0.42              |
| 36:1:3186:A:O2'    | 46:L9:23:ARG:NH2   | 2.53                     | 0.42              |
| 36:1:3254:G:O6     | 86:1:4059:OHX:N5   | 2.53                     | 0.42              |
| 86:1:4136:OHX:N3   | 86:1:4194:OHX:N4   | 2.66                     | 0.42              |
| 39:L2:104:LEU:HB3  | 39:L2:146:THR:HG21 | 2.02                     | 0.42              |
| 39:L2:245:LEU:HD23 | 39:L2:247:ARG:NH1  | 2.33                     | 0.42              |
| 43:L6:47:PHE:O     | 43:L6:50:LYS:HB2   | 2.20                     | 0.42              |
| 44:L7:106:LEU:HD23 | 44:L7:106:LEU:HA   | 1.83                     | 0.42              |
| 44:L7:175:LYS:HB3  | 44:L7:175:LYS:HE2  | 1.68                     | 0.42              |
| 45:L8:182:GLY:O    | 45:L8:186:LEU:HG   | 2.20                     | 0.42              |
| 45:L8:246:MET:HB2  | 45:L8:246:MET:HE3  | 1.80                     | 0.42              |
| 57:N1:12:ARG:HD3   | 57:N1:13:TYR:CZ    | 2.55                     | 0.42              |
| 61:N5:91:ASN:OD1   | 61:N5:94:GLN:HG3   | 2.20                     | 0.42              |
| 61:N5:92:LYS:HE2   | 61:N5:110:VAL:O    | 2.20                     | 0.42              |
| 62:N6:3:LYS:HE2    | 62:N6:8:VAL:O      | 2.20                     | 0.42              |
| 74:O8:59:ALA:O     | 74:O8:62:ALA:HB3   | 2.20                     | 0.42              |
| 1:6:470:A:C5'      | 1:6:470:A:C8       | 3.03                     | 0.42              |
| 1:6:1080:U:H3      | 1:6:1091:A:H2      | 1.66                     | 0.42              |
| 1:6:1082:C:C2'     | 1:6:1083:G:H5'     | 2.50                     | 0.42              |
| 1:6:1144:U:H2'     | 1:6:1145:U:C6      | 2.54                     | 0.42              |
| 1:6:1731:A:H5''    | 1:6:1732:A:OP2     | 2.20                     | 0.42              |
| 1:6:1740:A:H2'     | 1:6:1741:U:C6      | 2.55                     | 0.42              |
| 4:s2:40:LYS:HB2    | 4:s2:40:LYS:HE3    | 1.77                     | 0.42              |
| 7:s5:20:PHE:CE1    | 7:s5:34:GLN:HB3    | 2.55                     | 0.42              |
| 9:s7:91:ILE:HD11   | 9:s7:128:ASP:O     | 2.20                     | 0.42              |
| 9:s7:185:ILE:HG22  | 9:s7:186:PRO:HD3   | 2.01                     | 0.42              |
| 19:c7:34:LEU:O     | 19:c7:38:ILE:HD13  | 2.20                     | 0.42              |
| 31:d9:19:ARG:CD    | 31:d9:32:ARG:HD2   | 2.50                     | 0.42              |
| 34:sR:307:ASP:OD2  | 34:sR:311:ARG:NH2  | 2.42                     | 0.42              |
| 35:sM:37:VAL:HG12  | 35:sM:38:PRO:O     | 2.20                     | 0.42              |
| 36:5:221:A:H61     | 62:n6:103:LYS:NZ   | 2.18                     | 0.42              |
| 36:5:243:G:H2'     | 36:5:244:G:C8      | 2.55                     | 0.42              |
| 36:5:300:G:O6      | 86:5:4189:OHX:N2   | 2.53                     | 0.42              |
| 36:5:419:G:O3'     | 36:5:420:G:OP2     | 2.31                     | 0.42              |
| 36:5:523:A:N6      | 36:5:570:A:C2      | 2.88                     | 0.42              |
| 36:5:989:A:O2'     | 57:n1:104:GLU:HG2  | 2.20                     | 0.42              |
| 36:5:1111:U:O2'    | 36:5:1112:A:H5'    | 2.20                     | 0.42              |
| 36:5:1686:U:O4     | 58:n2:82:LYS:NZ    | 2.44                     | 0.42              |
| 36:5:1795:U:H2'    | 39:l2:50:HIS:CD2   | 2.54                     | 0.42              |
| 36:5:2943:G:C8     | 40:l3:2:SER:N      | 2.88                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 86:5:4065:OHX:N2   | 86:5:4074:OHX:N1  | 2.67                     | 0.42              |
| 86:5:4065:OHX:N4   | 86:5:4074:OHX:N1  | 2.67                     | 0.42              |
| 40:13:296:THR:HG21 | 40:13:357:LYS:C   | 2.44                     | 0.42              |
| 45:18:167:PRO:HB3  | 45:18:177:TYR:CZ  | 2.55                     | 0.42              |
| 47:m0:191:LYS:NZ   | 47:m0:212:GLU:HG3 | 2.35                     | 0.42              |
| 61:n5:67:ILE:HB    | 61:n5:83:VAL:HG12 | 2.00                     | 0.42              |
| 65:n9:36:ASP:CG    | 65:n9:38:LYS:O    | 2.63                     | 0.42              |
| 65:n9:40:ARG:HE    | 65:n9:40:ARG:HB3  | 1.76                     | 0.42              |
| 69:o3:10:LYS:O     | 69:o3:33:GLU:HB2  | 2.20                     | 0.42              |
| 74:o8:32:ASN:ND2   | 74:o8:34:ALA:HB3  | 2.34                     | 0.42              |
| 1:2:980:G:H4'      | 1:2:1776:A:H4'    | 2.02                     | 0.42              |
| 1:2:1063:U:OP1     | 29:D7:72:LYS:NZ   | 2.52                     | 0.42              |
| 1:2:1291:G:N2      | 1:2:1324:G:H22    | 2.16                     | 0.42              |
| 1:2:1417:A:OP1     | 86:2:2072:OHX:N5  | 2.53                     | 0.42              |
| 1:2:1475:A:H2'     | 1:2:1476:C:O4'    | 2.19                     | 0.42              |
| 1:2:1628:U:H2'     | 1:2:1629:G:C8     | 2.55                     | 0.42              |
| 9:S7:148:LYS:O     | 9:S7:149:ILE:HG13 | 2.19                     | 0.42              |
| 12:C0:88:PRO:C     | 12:C0:90:THR:H    | 2.28                     | 0.42              |
| 14:C2:33:ARG:HG2   | 14:C2:36:LEU:HD12 | 2.01                     | 0.42              |
| 17:C5:87:PRO:HA    | 17:C5:90:ILE:HG13 | 2.01                     | 0.42              |
| 18:C6:36:ILE:O     | 18:C6:36:ILE:HG12 | 2.20                     | 0.42              |
| 34:SR:192:PHE:HD1  | 34:SR:223:TRP:CE3 | 2.37                     | 0.42              |
| 35:SM:89:ARG:HD2   | 35:SM:89:ARG:O    | 2.20                     | 0.42              |
| 36:1:40:A:N7       | 64:N8:29:PRO:O    | 2.53                     | 0.42              |
| 36:1:551:A:O2'     | 36:1:552:G:O5'    | 2.28                     | 0.42              |
| 36:1:663:C:H2'     | 36:1:664:U:C6     | 2.55                     | 0.42              |
| 36:1:913:A:H2      | 36:1:2134:G:N3    | 2.18                     | 0.42              |
| 36:1:1316:C:O4'    | 52:M6:130:LYS:HD3 | 2.19                     | 0.42              |
| 36:1:1507:G:N7     | 53:M7:129:THR:CG2 | 2.82                     | 0.42              |
| 36:1:1724:U:OP2    | 55:M9:128:LYS:NZ  | 2.53                     | 0.42              |
| 36:1:1741:A:C2     | 36:1:1742:U:C4    | 3.08                     | 0.42              |
| 36:1:1767:C:C2'    | 36:1:1768:U:H5'   | 2.50                     | 0.42              |
| 36:1:2105:G:H2'    | 36:1:2106:A:H5'   | 2.00                     | 0.42              |
| 36:1:2118:C:O5'    | 36:1:2118:C:H6    | 2.03                     | 0.42              |
| 36:1:2775:U:H2'    | 36:1:2776:C:C6    | 2.55                     | 0.42              |
| 36:1:2896:A:H5'    | 36:1:2896:A:C8    | 2.55                     | 0.42              |
| 36:1:2899:C:C5     | 46:L9:171:ASP:HA  | 2.54                     | 0.42              |
| 36:1:2943:G:H2'    | 36:1:2944:U:O4'   | 2.20                     | 0.42              |
| 38:4:148:G:H2'     | 38:4:149:A:C8     | 2.55                     | 0.42              |
| 39:L2:181:LYS:HG3  | 39:L2:184:ARG:HG3 | 2.01                     | 0.42              |
| 42:L5:204:VAL:O    | 42:L5:208:MET:HG3 | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:L6:50:LYS:HG2  | 43:L6:74:VAL:HG21  | 2.02                     | 0.42              |
| 45:L8:148:ALA:HA  | 45:L8:201:THR:HG22 | 2.02                     | 0.42              |
| 51:M5:65:ARG:HD2  | 51:M5:129:TYR:CE1  | 2.55                     | 0.42              |
| 53:M7:36:ILE:CD1  | 53:M7:95:LEU:HD11  | 2.48                     | 0.42              |
| 54:M8:102:ALA:HB2 | 54:M8:122:ILE:HG22 | 2.02                     | 0.42              |
| 57:N1:119:ALA:HB2 | 57:N1:126:VAL:HG13 | 2.02                     | 0.42              |
| 64:N8:91:LEU:HD13 | 64:N8:91:LEU:HA    | 1.94                     | 0.42              |
| 69:O3:14:LEU:HD11 | 69:O3:31:LYS:HB2   | 2.01                     | 0.42              |
| 71:O5:44:ILE:O    | 71:O5:47:VAL:HG12  | 2.19                     | 0.42              |
| 73:O7:45:ARG:HE   | 73:O7:45:ARG:HB3   | 1.60                     | 0.42              |
| 74:O8:11:PHE:O    | 74:O8:14:LEU:HB2   | 2.19                     | 0.42              |
| 1:6:646:C:H2'     | 1:6:647:G:C8       | 2.55                     | 0.42              |
| 1:6:1241:G:OP1    | 17:c5:77:ARG:NH1   | 2.53                     | 0.42              |
| 1:6:1253:U:H4'    | 33:e1:143:LYS:N    | 2.35                     | 0.42              |
| 4:s2:41:LEU:HD23  | 4:s2:41:LEU:HA     | 1.84                     | 0.42              |
| 7:s5:35:GLN:C     | 7:s5:37:GLN:N      | 2.77                     | 0.42              |
| 8:s6:71:THR:HG22  | 8:s6:72:ARG:N      | 2.30                     | 0.42              |
| 12:c0:46:LEU:O    | 12:c0:50:THR:HG23  | 2.20                     | 0.42              |
| 27:d5:61:SER:OG   | 27:d5:62:VAL:N     | 2.53                     | 0.42              |
| 33:e1:113:LYS:HE3 | 33:e1:113:LYS:HB3  | 1.86                     | 0.42              |
| 34:sR:161:LYS:HE3 | 34:sR:161:LYS:HB3  | 1.83                     | 0.42              |
| 34:sR:283:LYS:HG3 | 34:sR:284:ALA:N    | 2.35                     | 0.42              |
| 36:5:287:G:H5'    | 51:m5:179:LYS:O    | 2.20                     | 0.42              |
| 36:5:769:G:O2'    | 49:m3:168:ARG:NH2  | 2.53                     | 0.42              |
| 36:5:1329:U:HO2'  | 36:5:1330:A:P      | 2.43                     | 0.42              |
| 36:5:1566:A:H2'   | 36:5:1567:U:H5'    | 2.02                     | 0.42              |
| 36:5:2138:A:O2'   | 73:o7:3:LYS:HG2    | 2.20                     | 0.42              |
| 36:5:2148:U:O2'   | 39:l2:182:ALA:HB2  | 2.20                     | 0.42              |
| 36:5:2434:U:H4'   | 36:5:2435:G:H5''   | 2.00                     | 0.42              |
| 36:5:2694:A:C6    | 36:5:2695:A:C6     | 3.08                     | 0.42              |
| 36:5:2729:U:H4'   | 54:m8:157:PRO:CB   | 2.49                     | 0.42              |
| 36:5:3163:A:O2'   | 36:5:3164:C:H5'    | 2.20                     | 0.42              |
| 38:8:113:U:H5''   | 75:o9:7:PHE:HB3    | 2.01                     | 0.42              |
| 38:8:157:U:O2'    | 38:8:158:U:H5'     | 2.19                     | 0.42              |
| 40:l3:86:VAL:HG22 | 40:l3:162:VAL:HG12 | 2.02                     | 0.42              |
| 41:l4:144:LYS:HD2 | 41:l4:145:ILE:HG22 | 2.01                     | 0.42              |
| 41:l4:329:PRO:HB2 | 41:l4:330:TYR:H    | 1.63                     | 0.42              |
| 46:l9:25:VAL:HG11 | 46:l9:78:MET:HE1   | 2.02                     | 0.42              |
| 62:n6:97:ILE:HG22 | 62:n6:99:LEU:HG    | 2.02                     | 0.42              |
| 72:o6:25:LYS:HE3  | 72:o6:25:LYS:HB3   | 1.87                     | 0.42              |
| 78:q2:14:GLY:O    | 78:q2:17:CYS:O     | 2.37                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:220:A:C6       | 1:2:221:A:N7       | 2.88                     | 0.41              |
| 1:2:434:G:N2       | 1:2:436:A:H3'      | 2.35                     | 0.41              |
| 1:2:709:C:N4       | 1:2:710:U:H1'      | 2.35                     | 0.41              |
| 1:2:1102:G:OP1     | 24:D2:76:SER:HB2   | 2.19                     | 0.41              |
| 1:2:1250:U:O2'     | 33:E1:135:HIS:HD2  | 2.03                     | 0.41              |
| 2:S0:123:VAL:HG11  | 2:S0:133:ILE:HD11  | 2.02                     | 0.41              |
| 3:S1:179:SER:HB3   | 3:S1:183:GLN:HB2   | 2.01                     | 0.41              |
| 4:S2:242:ILE:HD12  | 4:S2:242:ILE:HA    | 1.85                     | 0.41              |
| 11:S9:109:LEU:HD22 | 11:S9:113:VAL:HG23 | 2.02                     | 0.41              |
| 11:S9:158:PHE:CD2  | 11:S9:164:PHE:HB3  | 2.55                     | 0.41              |
| 14:C2:41:LEU:HD21  | 14:C2:123:VAL:HG22 | 2.02                     | 0.41              |
| 15:C3:53:LEU:HD12  | 15:C3:53:LEU:HA    | 1.74                     | 0.41              |
| 26:D4:52:LYS:C     | 26:D4:54:ALA:H     | 2.28                     | 0.41              |
| 27:D5:85:LYS:HG3   | 27:D5:86:GLU:N     | 2.33                     | 0.41              |
| 30:D8:27:GLN:CD    | 30:D8:64:ARG:HH21  | 2.27                     | 0.41              |
| 34:SR:286:GLU:HA   | 34:SR:287:PRO:HD3  | 1.66                     | 0.41              |
| 36:1:92:G:O5'      | 78:Q2:46:LYS:NZ    | 2.53                     | 0.41              |
| 36:1:1313:G:O6     | 86:1:4095:OHX:N3   | 2.53                     | 0.41              |
| 36:1:1814:A:OP1    | 86:1:4094:OHX:N2   | 2.53                     | 0.41              |
| 36:1:2947:G:OP2    | 36:1:2947:G:H4'    | 2.19                     | 0.41              |
| 86:1:3964:OHX:N2   | 86:1:4143:OHX:N6   | 2.68                     | 0.41              |
| 86:1:3980:OHX:N5   | 86:1:4158:OHX:N6   | 2.68                     | 0.41              |
| 37:3:26:C:H5''     | 42:L5:56:THR:HB    | 2.02                     | 0.41              |
| 40:L3:291:GLU:O    | 40:L3:292:ALA:HB3  | 2.19                     | 0.41              |
| 42:L5:178:ASN:O    | 42:L5:179:ARG:HD3  | 2.20                     | 0.41              |
| 42:L5:294:ALA:C    | 42:L5:296:GLN:N    | 2.77                     | 0.41              |
| 45:L8:45:ASN:CG    | 61:N5:26:VAL:HG23  | 2.45                     | 0.41              |
| 45:L8:77:GLN:C     | 45:L8:78:PHE:O     | 2.62                     | 0.41              |
| 45:L8:134:TYR:CD2  | 45:L8:190:VAL:HG21 | 2.55                     | 0.41              |
| 47:M0:216:TYR:CD2  | 47:M0:217:PHE:N    | 2.81                     | 0.41              |
| 54:M8:185:LYS:HD3  | 54:M8:186:VAL:HG23 | 2.01                     | 0.41              |
| 67:O1:16:LEU:HD12  | 67:O1:16:LEU:HA    | 1.79                     | 0.41              |
| 1:6:733:A:H2'      | 1:6:734:A:O4'      | 2.20                     | 0.41              |
| 1:6:1363:U:H3'     | 1:6:1364:G:H8      | 1.84                     | 0.41              |
| 1:6:1366:U:OP1     | 18:c6:30:LYS:HD3   | 2.20                     | 0.41              |
| 1:6:1535:U:HO2'    | 1:6:1536:G:P       | 2.43                     | 0.41              |
| 1:6:1573:A:H4'     | 1:6:1574:G:H5'     | 2.02                     | 0.41              |
| 2:s0:82:GLY:O      | 2:s0:86:VAL:HG22   | 2.19                     | 0.41              |
| 6:s4:11:ARG:O      | 6:s4:12:LEU:HB2    | 2.20                     | 0.41              |
| 11:s9:44:ARG:HG2   | 11:s9:45:ILE:HD13  | 2.02                     | 0.41              |
| 13:c1:86:ILE:HD11  | 13:c1:125:VAL:HG11 | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:c2:42:ALA:HB1   | 14:c2:47:GLU:HB3   | 2.02                     | 0.41              |
| 24:d2:73:GLY:HA3   | 24:d2:128:PHE:CZ   | 2.55                     | 0.41              |
| 34:sR:182:ASN:ND2  | 34:sR:184:ASN:HD21 | 2.18                     | 0.41              |
| 36:5:217:U:O2'     | 36:5:218:G:OP1     | 2.36                     | 0.41              |
| 36:5:289:A:H2      | 51:m5:93:LYS:HG3   | 1.85                     | 0.41              |
| 36:5:629:U:H2'     | 36:5:630:A:H8      | 1.81                     | 0.41              |
| 36:5:1001:G:H5'    | 36:5:1002:A:O5'    | 2.20                     | 0.41              |
| 36:5:1470:U:H2'    | 36:5:1471:U:H6     | 1.84                     | 0.41              |
| 36:5:2991:A:C2     | 53:m7:69:ARG:NH2   | 2.88                     | 0.41              |
| 86:5:4065:OHX:N6   | 86:5:4074:OHX:N5   | 2.68                     | 0.41              |
| 86:5:4212:OHX:N2   | 86:5:4222:OHX:N6   | 2.67                     | 0.41              |
| 37:7:79:A:C2       | 37:7:102:A:C4      | 3.08                     | 0.41              |
| 40:l3:227:GLU:HG3  | 40:l3:270:ARG:CB   | 2.50                     | 0.41              |
| 40:l3:380:MET:HB3  | 40:l3:380:MET:HE2  | 1.69                     | 0.41              |
| 41:l4:57:GLY:HA3   | 41:l4:98:ARG:H     | 1.85                     | 0.41              |
| 44:l7:131:GLU:HG2  | 44:l7:230:GLY:HA2  | 2.02                     | 0.41              |
| 46:l9:106:LYS:HG3  | 46:l9:107:ASP:OD2  | 2.20                     | 0.41              |
| 51:m5:143:ARG:HH21 | 71:o5:92:LEU:HA    | 1.85                     | 0.41              |
| 54:m8:122:ILE:HD13 | 54:m8:122:ILE:HG21 | 1.74                     | 0.41              |
| 55:m9:24:LEU:HD22  | 55:m9:50:ILE:HG12  | 2.02                     | 0.41              |
| 57:n1:120:LYS:C    | 57:n1:122:GLN:H    | 2.27                     | 0.41              |
| 62:n6:120:GLN:HE22 | 62:n6:126:LEU:N    | 2.18                     | 0.41              |
| 69:o3:100:ILE:N    | 69:o3:100:ILE:HD12 | 2.35                     | 0.41              |
| 72:o6:9:ILE:HG12   | 72:o6:10:GLY:N     | 2.35                     | 0.41              |
| 82:p0:25:LEU:HD21  | 82:p0:76:LEU:HD11  | 2.02                     | 0.41              |
| 82:p0:43:LYS:HB2   | 82:p0:43:LYS:HE3   | 1.87                     | 0.41              |
| 1:2:38:C:H2'       | 1:2:39:A:H5'       | 2.01                     | 0.41              |
| 1:2:196:G:O2'      | 1:2:197:A:P        | 2.78                     | 0.41              |
| 1:2:542:A:O2'      | 1:2:543:C:P        | 2.77                     | 0.41              |
| 1:2:710:U:H2'      | 1:2:711:U:H5'      | 2.03                     | 0.41              |
| 10:S8:36:THR:HA    | 10:S8:58:LEU:HA    | 2.00                     | 0.41              |
| 18:C6:5:PRO:HB3    | 18:C6:96:TYR:CE1   | 2.55                     | 0.41              |
| 18:C6:115:THR:HB   | 18:C6:118:ILE:O    | 2.20                     | 0.41              |
| 19:C7:119:LEU:H    | 19:C7:119:LEU:HD12 | 1.85                     | 0.41              |
| 33:E1:98:VAL:HG13  | 33:E1:99:LYS:N     | 2.34                     | 0.41              |
| 36:1:20:A:P        | 71:O5:90:ARG:HH11  | 2.42                     | 0.41              |
| 36:1:67:A:OP1      | 86:1:3915:OHX:N6   | 2.53                     | 0.41              |
| 36:1:402:A:C6      | 53:M7:21:TYR:CE2   | 3.08                     | 0.41              |
| 36:1:1100:U:OP2    | 44:L7:196:LYS:HE3  | 2.20                     | 0.41              |
| 36:1:1168:U:OP1    | 44:L7:211:SER:O    | 2.38                     | 0.41              |
| 36:1:1522:U:H4'    | 36:1:1523:U:OP2    | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:2320:A:C2    | 79:Q3:16:VAL:HG13  | 2.55                     | 0.41              |
| 36:1:2964:G:N7    | 86:1:4068:OHX:N3   | 2.68                     | 0.41              |
| 39:L2:48:ILE:HD11 | 79:Q3:54:ILE:HG23  | 2.02                     | 0.41              |
| 40:L3:3:HIS:O     | 40:L3:3:HIS:ND1    | 2.53                     | 0.41              |
| 40:L3:212:ASN:OD1 | 40:L3:354:VAL:HG22 | 2.20                     | 0.41              |
| 40:L3:313:HIS:O   | 40:L3:333:LYS:HD2  | 2.19                     | 0.41              |
| 41:L4:91:GLY:HA3  | 41:L4:93:MET:CE    | 2.48                     | 0.41              |
| 42:L5:180:PHE:HB3 | 42:L5:195:LEU:HD13 | 2.01                     | 0.41              |
| 46:L9:7:GLU:OE1   | 46:L9:54:LYS:HE3   | 2.20                     | 0.41              |
| 46:L9:57:VAL:HG23 | 46:L9:68:LEU:HG    | 2.03                     | 0.41              |
| 48:M1:89:TYR:O    | 48:M1:169:ALA:HB1  | 2.19                     | 0.41              |
| 51:M5:48:ALA:C    | 51:M5:53:TYR:HB3   | 2.45                     | 0.41              |
| 51:M5:175:ASN:O   | 51:M5:184:LYS:HG3  | 2.20                     | 0.41              |
| 59:N3:10:LYS:HG2  | 59:N3:11:PHE:O     | 2.20                     | 0.41              |
| 63:N7:108:GLU:HG2 | 63:N7:108:GLU:H    | 1.47                     | 0.41              |
| 76:Q0:110:CYS:SG  | 76:Q0:112:LYS:HB2  | 2.60                     | 0.41              |
| 79:Q3:27:LYS:O    | 79:Q3:31:ILE:HD12  | 2.20                     | 0.41              |
| 1:6:114:C:H6      | 1:6:114:C:H5'      | 1.85                     | 0.41              |
| 1:6:194:U:O2      | 1:6:194:U:H2'      | 2.19                     | 0.41              |
| 1:6:647:G:N2      | 1:6:687:G:N2       | 2.52                     | 0.41              |
| 1:6:919:A:H2'     | 1:6:920:U:C6       | 2.55                     | 0.41              |
| 1:6:1541:G:C6     | 1:6:1542:G:N1      | 2.88                     | 0.41              |
| 2:s0:69:ASN:HB3   | 2:s0:71:GLU:CD     | 2.45                     | 0.41              |
| 4:s2:116:LYS:HE3  | 4:s2:117:THR:O     | 2.20                     | 0.41              |
| 7:s5:94:THR:O     | 7:s5:97:LEU:HB2    | 2.20                     | 0.41              |
| 7:s5:156:ARG:HA   | 7:s5:157:ARG:HH21  | 1.84                     | 0.41              |
| 16:c4:91:THR:O    | 16:c4:93:THR:N     | 2.52                     | 0.41              |
| 21:c9:117:SER:HB2 | 21:c9:123:ARG:HB3  | 2.01                     | 0.41              |
| 24:d2:37:PHE:HD1  | 24:d2:41:MET:HE2   | 1.85                     | 0.41              |
| 36:5:209:A:H4'    | 36:5:211:A:N7      | 2.34                     | 0.41              |
| 36:5:409:A:OP2    | 86:5:4102:OHX:N3   | 2.53                     | 0.41              |
| 36:5:529:A:H2'    | 36:5:530:G:O4'     | 2.20                     | 0.41              |
| 36:5:1283:C:OP1   | 82:p0:81:LYS:HD3   | 2.20                     | 0.41              |
| 36:5:1456:A:N1    | 67:o1:64:VAL:HG13  | 2.35                     | 0.41              |
| 36:5:1721:U:OP2   | 55:m9:124:TYR:OH   | 2.38                     | 0.41              |
| 36:5:1729:A:H4'   | 36:5:1730:G:OP2    | 2.19                     | 0.41              |
| 36:5:2529:A:H2'   | 36:5:2530:G:O4'    | 2.21                     | 0.41              |
| 36:5:2895:G:H5'   | 36:5:3107:U:O2'    | 2.20                     | 0.41              |
| 36:5:2965:U:O2    | 39:l2:221:LYS:NZ   | 2.43                     | 0.41              |
| 36:5:3219:G:H4'   | 36:5:3220:G:H5'    | 2.02                     | 0.41              |
| 36:5:3269:U:H5'   | 36:5:3271:G:O4'    | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:3269:U:O2     | 36:5:3271:G:N1     | 2.53                     | 0.41              |
| 37:7:112:G:OP2     | 86:7:221:OHX:N2    | 2.52                     | 0.41              |
| 39:12:48:ILE:HG12  | 79:q3:63:THR:CG2   | 2.49                     | 0.41              |
| 41:l4:302:ALA:HB2  | 54:m8:39:ARG:NH1   | 2.35                     | 0.41              |
| 44:l7:26:VAL:C     | 44:l7:28:ALA:H     | 2.28                     | 0.41              |
| 45:l8:75:ILE:HG13  | 51:m5:18:VAL:HG23  | 2.01                     | 0.41              |
| 47:m0:215:GLU:CD   | 47:m0:215:GLU:H    | 2.27                     | 0.41              |
| 48:m1:37:LEU:HD13  | 48:m1:69:VAL:HG12  | 2.02                     | 0.41              |
| 81:m2:116:UNK:O    | 81:m2:118:UNK:N    | 2.52                     | 0.41              |
| 61:n5:82:LEU:HD21  | 61:n5:135:ILE:CG2  | 2.50                     | 0.41              |
| 61:n5:103:TYR:O    | 61:n5:138:ARG:NH1  | 2.53                     | 0.41              |
| 61:n5:103:TYR:HB3  | 61:n5:135:ILE:HD11 | 2.00                     | 0.41              |
| 62:n6:56:VAL:O     | 62:n6:67:GLU:HA    | 2.20                     | 0.41              |
| 63:n7:135:ARG:HH21 | 63:n7:135:ARG:CB   | 2.28                     | 0.41              |
| 64:n8:73:LEU:HD11  | 64:n8:78:LEU:HA    | 2.02                     | 0.41              |
| 69:o3:85:PHE:CZ    | 69:o3:89:LEU:HD11  | 2.54                     | 0.41              |
| 86:2:2084:OHX:N3   | 86:2:2086:OHX:N1   | 2.67                     | 0.41              |
| 4:S2:44:LEU:HD23   | 4:S2:44:LEU:HA     | 1.86                     | 0.41              |
| 6:S4:21:ASP:OD1    | 6:S4:24:SER:OG     | 2.38                     | 0.41              |
| 6:S4:87:MET:O      | 6:S4:122:LYS:HE3   | 2.21                     | 0.41              |
| 6:S4:194:THR:O     | 6:S4:195:ILE:CB    | 2.68                     | 0.41              |
| 7:S5:53:VAL:CG2    | 7:S5:59:VAL:HG22   | 2.50                     | 0.41              |
| 7:S5:188:LYS:HE2   | 7:S5:196:GLU:OE2   | 2.20                     | 0.41              |
| 9:S7:12:ALA:HB3    | 9:S7:13:PRO:HD3    | 2.01                     | 0.41              |
| 9:S7:70:PHE:O      | 9:S7:74:GLN:HB2    | 2.19                     | 0.41              |
| 10:S8:169:ILE:HD12 | 10:S8:179:CYS:SG   | 2.61                     | 0.41              |
| 16:C4:19:ILE:HD11  | 16:C4:105:LEU:HD21 | 2.02                     | 0.41              |
| 21:C9:89:ARG:HH11  | 21:C9:89:ARG:HG3   | 1.84                     | 0.41              |
| 28:D6:40:ALA:HB2   | 28:D6:71:LEU:HD21  | 2.01                     | 0.41              |
| 35:SM:63:ASP:C     | 35:SM:64:LYS:O     | 2.63                     | 0.41              |
| 36:1:510:G:O6      | 86:1:4011:OHX:N1   | 2.53                     | 0.41              |
| 36:1:1769:G:O6     | 86:1:4172:OHX:N4   | 2.53                     | 0.41              |
| 36:1:2209:U:H6     | 36:1:2209:U:H2'    | 1.70                     | 0.41              |
| 36:1:2408:U:O2'    | 36:1:2409:G:H5'    | 2.20                     | 0.41              |
| 36:1:2599:U:H2'    | 36:1:2600:C:C6     | 2.55                     | 0.41              |
| 36:1:2768:U:H2'    | 36:1:2769:A:C8     | 2.55                     | 0.41              |
| 36:1:3020:U:OP2    | 36:1:3021:A:O2'    | 2.38                     | 0.41              |
| 36:1:3181:C:H2'    | 36:1:3182:G:O4'    | 2.21                     | 0.41              |
| 86:1:4144:OHX:N1   | 86:1:4187:OHX:N5   | 2.68                     | 0.41              |
| 37:3:19:C:H2'      | 37:3:20:A:C8       | 2.55                     | 0.41              |
| 38:4:143:U:H2'     | 38:4:144:G:O4'     | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:L3:169:THR:CG2  | 40:L3:171:LEU:H    | 2.33                     | 0.41              |
| 42:L5:40:HIS:HD2   | 42:L5:42:ALA:N     | 2.07                     | 0.41              |
| 44:L7:116:PHE:CZ   | 44:L7:144:ILE:HG12 | 2.55                     | 0.41              |
| 45:L8:100:GLU:OE1  | 45:L8:108:ARG:NH1  | 2.50                     | 0.41              |
| 47:M0:24:ARG:HH11  | 47:M0:24:ARG:CG    | 2.26                     | 0.41              |
| 47:M0:34:TYR:N     | 47:M0:34:TYR:CD1   | 2.89                     | 0.41              |
| 50:M4:37:GLU:HG2   | 56:N0:72:VAL:HG21  | 2.02                     | 0.41              |
| 53:M7:26:PHE:CE1   | 53:M7:120:ASN:HA   | 2.55                     | 0.41              |
| 55:M9:44:LEU:HD12  | 55:M9:44:LEU:HA    | 1.83                     | 0.41              |
| 56:N0:44:PHE:CD1   | 57:N1:153:PRO:HG3  | 2.55                     | 0.41              |
| 56:N0:45:LEU:HD12  | 56:N0:49:HIS:HB2   | 2.01                     | 0.41              |
| 67:O1:55:LEU:HB2   | 67:O1:95:PRO:HD3   | 2.01                     | 0.41              |
| 71:O5:100:VAL:HG22 | 71:O5:104:GLN:HB3  | 2.03                     | 0.41              |
| 75:O9:9:ILE:HG22   | 75:O9:13:MET:HE2   | 2.02                     | 0.41              |
| 1:6:1001:A:C6      | 1:6:1002:G:C6      | 3.09                     | 0.41              |
| 1:6:1029:U:O2'     | 1:6:1030:A:H5'     | 2.21                     | 0.41              |
| 1:6:1280:C:O2'     | 22:d0:70:THR:HG23  | 2.20                     | 0.41              |
| 1:6:1685:G:H1      | 1:6:1716:C:N4      | 2.18                     | 0.41              |
| 3:s1:130:SER:OG    | 3:s1:180:THR:HG22  | 2.20                     | 0.41              |
| 5:s3:168:ILE:HA    | 5:s3:188:ILE:O     | 2.21                     | 0.41              |
| 9:s7:39:ARG:HH22   | 55:m9:185:LEU:HD22 | 1.86                     | 0.41              |
| 11:s9:182:GLU:OE1  | 11:s9:183:ALA:N    | 2.54                     | 0.41              |
| 22:d0:36:ASN:HA    | 22:d0:39:SER:CB    | 2.51                     | 0.41              |
| 34:sR:45:TRP:CZ3   | 34:sR:57:PRO:HD3   | 2.55                     | 0.41              |
| 35:sM:52:PRO:C     | 35:sM:54:PRO:HD3   | 2.45                     | 0.41              |
| 36:5:113:C:C2      | 36:5:319:A:C2      | 3.08                     | 0.41              |
| 36:5:597:G:OP1     | 44:l7:37:ASN:HB3   | 2.21                     | 0.41              |
| 36:5:599:C:H2'     | 36:5:600:G:O4'     | 2.20                     | 0.41              |
| 36:5:1471:U:H4'    | 55:m9:3:ASN:OD1    | 2.20                     | 0.41              |
| 36:5:1481:A:O2'    | 36:5:1858:A:C2     | 2.65                     | 0.41              |
| 36:5:1650:G:N7     | 86:5:4179:OHX:N3   | 2.67                     | 0.41              |
| 36:5:2530:G:C2'    | 36:5:2531:C:H5'    | 2.50                     | 0.41              |
| 36:5:2875:U:C2'    | 36:5:2876:C:O5'    | 2.68                     | 0.41              |
| 36:5:3288:G:O2'    | 36:5:3289:G:P      | 2.78                     | 0.41              |
| 39:l2:113:VAL:HG23 | 39:l2:134:VAL:HG22 | 2.02                     | 0.41              |
| 40:l3:152:LYS:HD3  | 40:l3:189:SER:HA   | 2.03                     | 0.41              |
| 41:l4:3:ARG:HA     | 41:l4:4:PRO:HD3    | 1.75                     | 0.41              |
| 42:l5:21:ARG:O     | 42:l5:25:GLU:HG3   | 2.20                     | 0.41              |
| 43:l6:152:THR:HA   | 43:l6:153:PRO:HD3  | 1.92                     | 0.41              |
| 48:m1:60:ARG:NH1   | 78:q2:104:LEU:O    | 2.49                     | 0.41              |
| 51:m5:121:VAL:HG11 | 51:m5:131:GLU:HG3  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:m7:67:ILE:HD12 | 53:m7:82:ARG:NH1   | 2.35                     | 0.41              |
| 54:m8:170:ARG:HD2 | 64:n8:56:VAL:O     | 2.20                     | 0.41              |
| 58:n2:97:SER:HB2  | 58:n2:103:TYR:CE1  | 2.55                     | 0.41              |
| 60:n4:93:ARG:HD3  | 60:n4:93:ARG:HA    | 1.57                     | 0.41              |
| 63:n7:5:LEU:HD23  | 63:n7:25:ILE:CD1   | 2.50                     | 0.41              |
| 63:n7:97:SER:OG   | 63:n7:98:THR:N     | 2.52                     | 0.41              |
| 65:n9:39:PHE:CD2  | 65:n9:39:PHE:C     | 2.98                     | 0.41              |
| 67:o1:77:ARG:HA   | 67:o1:90:PHE:O     | 2.20                     | 0.41              |
| 68:o2:7:PRO:O     | 68:o2:8:LYS:C      | 2.61                     | 0.41              |
| 82:p0:37:GLN:HA   | 82:p0:104:ARG:HD2  | 2.01                     | 0.41              |
| 1:2:196:G:O2'     | 1:2:197:A:OP2      | 2.30                     | 0.41              |
| 1:2:209:U:H2'     | 1:2:210:A:C8       | 2.56                     | 0.41              |
| 1:2:1500:C:OP1    | 21:C9:122:ARG:NH2  | 2.50                     | 0.41              |
| 6:S4:114:ILE:HB   | 6:S4:118:GLU:OE2   | 2.20                     | 0.41              |
| 6:S4:199:GLU:HB2  | 6:S4:207:LEU:HB2   | 2.03                     | 0.41              |
| 9:S7:35:LYS:NZ    | 9:S7:36:ALA:H      | 2.18                     | 0.41              |
| 9:S7:39:ARG:HH12  | 55:M9:188:ASP:HB2  | 1.85                     | 0.41              |
| 10:S8:117:TYR:O   | 10:S8:119:GLN:HG2  | 2.20                     | 0.41              |
| 12:C0:33:GLU:O    | 12:C0:34:GLU:HB2   | 2.21                     | 0.41              |
| 13:C1:98:ASN:ND2  | 24:D2:79:PHE:CD1   | 2.89                     | 0.41              |
| 22:D0:18:GLN:O    | 22:D0:96:PRO:HA    | 2.20                     | 0.41              |
| 22:D0:63:LEU:HD22 | 31:D9:34:TYR:CE1   | 2.56                     | 0.41              |
| 25:D3:96:VAL:HG12 | 25:D3:127:VAL:HG11 | 2.02                     | 0.41              |
| 28:D6:4:LYS:HE2   | 28:D6:5:ARG:NH2    | 2.35                     | 0.41              |
| 33:E1:93:HIS:HB3  | 33:E1:94:LYS:H     | 1.46                     | 0.41              |
| 34:SR:40:LYS:HG2  | 34:SR:66:HIS:O     | 2.20                     | 0.41              |
| 36:1:255:A:O2'    | 36:1:256:G:H5'     | 2.21                     | 0.41              |
| 36:1:1211:U:H2'   | 36:1:1212:A:C8     | 2.55                     | 0.41              |
| 36:1:1247:U:H2'   | 36:1:1268:G:O6     | 2.19                     | 0.41              |
| 36:1:1565:G:N2    | 36:1:1574:C:C2     | 2.89                     | 0.41              |
| 36:1:2137:U:C6    | 36:1:2141:U:C4     | 3.09                     | 0.41              |
| 36:1:2261:G:O2'   | 36:1:2263:C:N4     | 2.53                     | 0.41              |
| 36:1:2356:A:O2'   | 53:M7:137:ASN:HB3  | 2.20                     | 0.41              |
| 86:1:4084:OHX:N6  | 86:1:4153:OHX:N3   | 2.68                     | 0.41              |
| 37:3:55:A:H2'     | 37:3:56:A:O4'      | 2.21                     | 0.41              |
| 38:4:141:C:O2'    | 38:4:142:C:H5'     | 2.19                     | 0.41              |
| 39:L2:206:PRO:C   | 39:L2:208:ASP:H    | 2.28                     | 0.41              |
| 40:L3:124:LYS:HB2 | 40:L3:124:LYS:HE3  | 1.81                     | 0.41              |
| 40:L3:159:ARG:HG2 | 40:L3:182:GLN:HA   | 2.02                     | 0.41              |
| 41:L4:208:VAL:O   | 41:L4:251:THR:HG23 | 2.21                     | 0.41              |
| 41:L4:274:TYR:CG  | 41:L4:275:THR:N    | 2.88                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:L5:110:LEU:HD13 | 42:L5:171:LEU:HD23 | 2.01                     | 0.41              |
| 42:L5:261:THR:HG23 | 42:L5:264:GLN:CD   | 2.46                     | 0.41              |
| 45:L8:84:ARG:HB3   | 45:L8:84:ARG:NH1   | 2.35                     | 0.41              |
| 49:M3:55:ARG:O     | 49:M3:115:ARG:NH2  | 2.34                     | 0.41              |
| 56:N0:7:TYR:CE1    | 56:N0:34:GLU:HG2   | 2.55                     | 0.41              |
| 66:O0:20:SER:OG    | 66:O0:97:ASP:N     | 2.52                     | 0.41              |
| 67:O1:80:ASN:OD1   | 67:O1:81:GLU:N     | 2.53                     | 0.41              |
| 1:6:282:C:H2'      | 1:6:283:U:O4'      | 2.20                     | 0.41              |
| 1:6:517:U:H2'      | 1:6:518:A:O4'      | 2.21                     | 0.41              |
| 1:6:604:A:OP2      | 86:6:2151:OHX:N4   | 2.54                     | 0.41              |
| 1:6:1229:G:O2'     | 1:6:1230:A:OP2     | 2.36                     | 0.41              |
| 1:6:1248:C:H2'     | 1:6:1249:U:C6      | 2.55                     | 0.41              |
| 1:6:1274:C:N3      | 1:6:1427:A:C8      | 2.88                     | 0.41              |
| 7:s5:25:LEU:HB2    | 18:c6:27:GLY:O     | 2.20                     | 0.41              |
| 7:s5:143:ARG:HD3   | 30:d8:55:VAL:HG11  | 2.01                     | 0.41              |
| 15:c3:142:GLU:O    | 15:c3:143:SER:C    | 2.63                     | 0.41              |
| 18:c6:54:LEU:HA    | 18:c6:54:LEU:HD13  | 1.75                     | 0.41              |
| 27:d5:49:ARG:HD2   | 27:d5:53:GLU:OE1   | 2.21                     | 0.41              |
| 30:d8:11:LYS:O     | 30:d8:30:VAL:HA    | 2.21                     | 0.41              |
| 36:5:29:C:H4'      | 36:5:62:A:H4'      | 2.02                     | 0.41              |
| 36:5:1017:C:H42    | 36:5:2671:A:P      | 2.44                     | 0.41              |
| 36:5:1143:A:H4'    | 36:5:1144:U:OP2    | 2.20                     | 0.41              |
| 36:5:1299:U:OP1    | 76:q0:113:ARG:NH1  | 2.53                     | 0.41              |
| 36:5:1646:G:N3     | 36:5:1808:G:C2     | 2.88                     | 0.41              |
| 37:7:8:G:C6        | 37:7:9:C:C4        | 3.09                     | 0.41              |
| 40:l3:37:ARG:O     | 40:l3:186:GLY:HA3  | 2.19                     | 0.41              |
| 41:l4:145:ILE:HA   | 41:l4:146:PRO:HD3  | 1.86                     | 0.41              |
| 57:n1:27:LEU:O     | 57:n1:28:SER:C     | 2.63                     | 0.41              |
| 57:n1:115:LYS:HB2  | 57:n1:128:LEU:HD21 | 2.02                     | 0.41              |
| 60:n4:55:PHE:CD1   | 60:n4:55:PHE:C     | 2.99                     | 0.41              |
| 61:n5:115:ARG:HH11 | 61:n5:115:ARG:CG   | 2.31                     | 0.41              |
| 62:n6:59:VAL:O     | 62:n6:64:LYS:HD2   | 2.21                     | 0.41              |
| 63:n7:70:PRO:HG3   | 63:n7:115:LYS:HB2  | 2.02                     | 0.41              |
| 64:n8:47:LYS:O     | 64:n8:48:TYR:HB2   | 2.21                     | 0.41              |
| 67:o1:41:LYS:HA    | 67:o1:46:THR:HG22  | 2.03                     | 0.41              |
| 72:o6:62:ARG:O     | 72:o6:63:ASN:ND2   | 2.48                     | 0.41              |
| 1:2:11:A:H4'       | 4:S2:87:GLN:HG3    | 2.03                     | 0.41              |
| 1:2:464:A:C2       | 1:2:465:G:C8       | 3.08                     | 0.41              |
| 1:2:768:C:C6       | 11:S9:143:ILE:HD13 | 2.56                     | 0.41              |
| 3:S1:89:ASP:OD1    | 3:S1:89:ASP:N      | 2.53                     | 0.41              |
| 3:S1:134:VAL:HB    | 3:S1:219:LYS:HB2   | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:S2:84:LYS:HA    | 4:S2:85:PRO:HD3   | 1.92                     | 0.41              |
| 7:S5:72:HIS:O     | 7:S5:73:THR:OG1   | 2.36                     | 0.41              |
| 7:S5:205:SER:O    | 7:S5:207:THR:HG23 | 2.20                     | 0.41              |
| 8:S6:71:THR:OG1   | 8:S6:72:ARG:N     | 2.52                     | 0.41              |
| 12:C0:77:ARG:HA   | 12:C0:82:LEU:CD1  | 2.50                     | 0.41              |
| 20:C8:86:LEU:HG   | 20:C8:99:HIS:HB2  | 2.03                     | 0.41              |
| 25:D3:12:ALA:O    | 25:D3:16:ARG:HG3  | 2.20                     | 0.41              |
| 35:SM:102:THR:CG2 | 35:SM:105:LYS:H   | 2.32                     | 0.41              |
| 36:1:147:U:O4     | 45:L8:157:VAL:HA  | 2.20                     | 0.41              |
| 36:1:243:G:H2'    | 36:1:244:G:O4'    | 2.20                     | 0.41              |
| 36:1:439:C:C4     | 36:1:440:A:C6     | 3.08                     | 0.41              |
| 36:1:528:U:H2'    | 36:1:529:A:C8     | 2.55                     | 0.41              |
| 36:1:1048:A:H2'   | 47:M0:22:TYR:CZ   | 2.55                     | 0.41              |
| 36:1:1325:U:H2'   | 36:1:1326:A:O4'   | 2.20                     | 0.41              |
| 36:1:1349:G:H3'   | 36:1:1349:G:N3    | 2.35                     | 0.41              |
| 36:1:1434:G:OP1   | 36:1:1437:C:N4    | 2.54                     | 0.41              |
| 42:L5:164:LYS:HG2 | 42:L5:180:PHE:CZ  | 2.55                     | 0.41              |
| 44:L7:159:GLN:O   | 44:L7:160:ARG:C   | 2.63                     | 0.41              |
| 51:M5:143:ARG:NH2 | 71:O5:92:LEU:HD23 | 2.34                     | 0.41              |
| 57:N1:68:THR:HG23 | 57:N1:69:LYS:N    | 2.36                     | 0.41              |
| 69:O3:13:HIS:HB3  | 69:O3:93:THR:O    | 2.21                     | 0.41              |
| 72:O6:60:LEU:HD13 | 72:O6:60:LEU:HA   | 1.79                     | 0.41              |
| 1:6:994:G:C2'     | 1:6:995:A:H5'     | 2.51                     | 0.41              |
| 1:6:1095:U:O4     | 86:6:2180:OHX:N2  | 2.54                     | 0.41              |
| 1:6:1553:G:O2'    | 31:d9:14:TYR:OH   | 2.35                     | 0.41              |
| 2:s0:74:VAL:HG23  | 2:s0:118:PRO:HB3  | 2.03                     | 0.41              |
| 3:s1:103:MET:HE2  | 3:s1:215:VAL:HG12 | 2.02                     | 0.41              |
| 6:s4:180:LEU:HD23 | 6:s4:180:LEU:HA   | 1.88                     | 0.41              |
| 6:s4:233:LYS:NZ   | 6:s4:235:TYR:HE2  | 2.18                     | 0.41              |
| 8:s6:48:TYR:CD2   | 8:s6:117:GLY:HA3  | 2.55                     | 0.41              |
| 8:s6:216:LEU:HD23 | 8:s6:216:LEU:HA   | 1.84                     | 0.41              |
| 36:5:371:G:O6     | 86:5:4203:OHX:N5  | 2.52                     | 0.41              |
| 36:5:578:A:H5''   | 36:5:579:G:O5'    | 2.21                     | 0.41              |
| 36:5:908:G:H4'    | 36:5:909:G:O5'    | 2.21                     | 0.41              |
| 36:5:1393:A:C8    | 36:5:1418:A:C6    | 3.09                     | 0.41              |
| 36:5:1817:G:O2'   | 36:5:1818:U:P     | 2.79                     | 0.41              |
| 36:5:1864:A:H2'   | 36:5:1865:A:C8    | 2.55                     | 0.41              |
| 36:5:2304:C:C5    | 36:5:2305:G:C6    | 3.08                     | 0.41              |
| 36:5:2403:G:N2    | 36:5:2404:A:C5    | 2.74                     | 0.41              |
| 36:5:2518:C:C2    | 36:5:2590:A:C2    | 3.09                     | 0.41              |
| 36:5:2947:G:C2    | 40:l3:250:ALA:HB1 | 2.56                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:5:3084:C:H2'   | 36:5:3085:G:O4'    | 2.20                     | 0.41              |
| 36:5:3243:A:C5    | 52:m6:156:LEU:HB3  | 2.56                     | 0.41              |
| 36:5:3288:G:O2'   | 36:5:3289:G:OP2    | 2.33                     | 0.41              |
| 37:7:27:A:H2'     | 37:7:28:C:C6       | 2.55                     | 0.41              |
| 37:7:91:G:H2'     | 37:7:92:A:C8       | 2.56                     | 0.41              |
| 39:l2:183:GLY:O   | 39:l2:186:PHE:HB3  | 2.20                     | 0.41              |
| 40:l3:183:LEU:HA  | 40:l3:183:LEU:HD12 | 1.70                     | 0.41              |
| 43:l6:131:LYS:HD3 | 43:l6:132:ALA:N    | 2.36                     | 0.41              |
| 45:l8:121:SER:O   | 45:l8:123:GLN:N    | 2.54                     | 0.41              |
| 48:m1:152:HIS:O   | 48:m1:153:LYS:HB3  | 2.21                     | 0.41              |
| 60:n4:126:GLU:HG2 | 60:n4:129:LYS:HZ2  | 1.84                     | 0.41              |
| 66:o0:83:LYS:HG2  | 66:o0:85:PHE:CZ    | 2.56                     | 0.41              |
| 70:o4:100:ILE:H   | 70:o4:100:ILE:HG13 | 1.71                     | 0.41              |
| 75:o9:21:ARG:HD3  | 75:o9:22:PRO:O     | 2.20                     | 0.41              |
| 82:p0:42:ARG:O    | 82:p0:46:ARG:HG2   | 2.21                     | 0.41              |
| 1:2:778:G:H22     | 26:D4:10:ARG:CZ    | 2.34                     | 0.41              |
| 1:2:927:C:H1'     | 16:C4:125:SER:HB2  | 2.01                     | 0.41              |
| 1:2:1287:A:H4'    | 1:2:1288:G:OP1     | 2.21                     | 0.41              |
| 2:S0:50:VAL:H     | 19:C7:109:LEU:HD21 | 1.86                     | 0.41              |
| 2:S0:185:ARG:H    | 23:D1:44:ARG:HA    | 1.85                     | 0.41              |
| 4:S2:111:VAL:HG21 | 4:S2:218:ILE:HD13  | 2.03                     | 0.41              |
| 4:S2:125:ILE:O    | 4:S2:129:ILE:HG13  | 2.20                     | 0.41              |
| 5:S3:64:ARG:O     | 5:S3:65:ARG:C      | 2.63                     | 0.41              |
| 7:S5:43:PHE:HA    | 7:S5:68:ILE:O      | 2.20                     | 0.41              |
| 7:S5:73:THR:HG23  | 18:C6:114:ARG:HG3  | 2.01                     | 0.41              |
| 9:S7:44:LYS:HG3   | 9:S7:63:PRO:HD3    | 2.02                     | 0.41              |
| 12:C0:80:LEU:O    | 12:C0:81:ASN:ND2   | 2.47                     | 0.41              |
| 15:C3:46:THR:N    | 15:C3:49:GLN:OE1   | 2.46                     | 0.41              |
| 15:C3:47:PRO:HG3  | 15:C3:75:LEU:HD22  | 2.02                     | 0.41              |
| 18:C6:10:PHE:CD1  | 18:C6:10:PHE:C     | 2.99                     | 0.41              |
| 36:1:65:A:C4      | 36:1:110:G:N7      | 2.88                     | 0.41              |
| 36:1:94:G:H2'     | 36:1:95:A:C8       | 2.56                     | 0.41              |
| 36:1:210:U:C2     | 36:1:230:U:H4'     | 2.56                     | 0.41              |
| 36:1:241:G:C6     | 36:1:242:C:C4      | 3.08                     | 0.41              |
| 36:1:362:U:OP1    | 73:O7:45:ARG:NH2   | 2.54                     | 0.41              |
| 36:1:508:U:H2'    | 36:1:509:U:C6      | 2.55                     | 0.41              |
| 36:1:1040:A:N3    | 47:M0:198:LYS:NZ   | 2.62                     | 0.41              |
| 36:1:1310:G:N7    | 86:1:4031:OHX:N5   | 2.68                     | 0.41              |
| 36:1:1522:U:H3'   | 61:N5:113:LEU:HD22 | 2.02                     | 0.41              |
| 36:1:1560:G:C2    | 36:1:1561:G:N7     | 2.89                     | 0.41              |
| 36:1:1947:G:H1    | 36:1:2101:C:N4     | 2.17                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:2523:A:H2'   | 45:L8:49:TYR:O     | 2.21                     | 0.41              |
| 36:1:2611:U:H2'   | 36:1:2612:U:H6     | 1.86                     | 0.41              |
| 86:1:4065:OHX:N6  | 86:1:4177:OHX:N2   | 2.68                     | 0.41              |
| 37:3:11:A:O2'     | 37:3:13:A:OP2      | 2.26                     | 0.41              |
| 38:4:9:A:H2'      | 38:4:10:A:C8       | 2.55                     | 0.41              |
| 38:4:79:A:C6      | 38:4:80:A:C2       | 3.09                     | 0.41              |
| 38:4:157:U:H3'    | 38:4:158:U:C6      | 2.56                     | 0.41              |
| 40:L3:305:ILE:H   | 40:L3:305:ILE:HG13 | 1.53                     | 0.41              |
| 41:L4:93:MET:HE3  | 41:L4:94:CYS:SG    | 2.60                     | 0.41              |
| 41:L4:304:GLN:C   | 41:L4:306:THR:H    | 2.29                     | 0.41              |
| 42:L5:59:ASP:OD1  | 42:L5:81:HIS:HD2   | 2.04                     | 0.41              |
| 43:L6:7:PRO:HG2   | 43:L6:10:TYR:CZ    | 2.56                     | 0.41              |
| 44:L7:158:LYS:CG  | 44:L7:159:GLN:N    | 2.81                     | 0.41              |
| 49:M3:138:VAL:HB  | 71:O5:118:ILE:HB   | 2.02                     | 0.41              |
| 53:M7:138:LYS:HG3 | 53:M7:140:GLU:HG3  | 2.03                     | 0.41              |
| 59:N3:119:GLY:HA2 | 59:N3:137:VAL:HG23 | 2.01                     | 0.41              |
| 61:N5:25:LYS:HD3  | 61:N5:27:ARG:NH1   | 2.35                     | 0.41              |
| 64:N8:74:ASN:HB3  | 64:N8:115:LYS:HB2  | 2.01                     | 0.41              |
| 65:N9:56:ALA:C    | 65:N9:58:LYS:H     | 2.29                     | 0.41              |
| 1:6:72:A:H2'      | 1:6:73:U:C1'       | 2.50                     | 0.41              |
| 1:6:754:A:N6      | 1:6:793:A:N7       | 2.67                     | 0.41              |
| 1:6:755:A:O2'     | 1:6:756:A:P        | 2.79                     | 0.41              |
| 1:6:846:G:N2      | 13:c1:46:LYS:HE2   | 2.35                     | 0.41              |
| 1:6:1050:G:N2     | 1:6:1068:C:O2      | 2.54                     | 0.41              |
| 1:6:1179:G:C6     | 1:6:1180:C:C4      | 3.08                     | 0.41              |
| 6:s4:23:LEU:O     | 6:s4:24:SER:CB     | 2.69                     | 0.41              |
| 6:s4:35:PRO:HB3   | 6:s4:143:ASP:O     | 2.21                     | 0.41              |
| 6:s4:128:LYS:HA   | 6:s4:156:VAL:HG22  | 2.01                     | 0.41              |
| 8:s6:4:ASN:HB3    | 8:s6:110:ALA:HA    | 2.02                     | 0.41              |
| 10:s8:21:PHE:HD1  | 10:s8:22:ARG:HG2   | 1.85                     | 0.41              |
| 11:s9:8:TYR:CD1   | 11:s9:8:TYR:C      | 2.99                     | 0.41              |
| 16:c4:47:LYS:HB3  | 16:c4:62:LEU:HD23  | 2.01                     | 0.41              |
| 21:c9:42:GLY:HA2  | 21:c9:84:LYS:HG3   | 2.03                     | 0.41              |
| 28:d6:62:TYR:CG   | 28:d6:63:ALA:N     | 2.81                     | 0.41              |
| 36:5:603:A:H2'    | 36:5:604:G:O4'     | 2.21                     | 0.41              |
| 36:5:608:A:N6     | 43:l6:22:ARG:HD3   | 2.36                     | 0.41              |
| 36:5:698:U:H2'    | 36:5:699:A:O4'     | 2.20                     | 0.41              |
| 36:5:1263:A:H2'   | 36:5:1263:A:N3     | 2.36                     | 0.41              |
| 36:5:2587:U:O2'   | 36:5:2588:U:H5'    | 2.20                     | 0.41              |
| 36:5:2590:A:C6    | 36:5:2591:A:C5     | 3.09                     | 0.41              |
| 36:5:2736:A:OP1   | 57:n1:92:ARG:NH1   | 2.50                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:2872:A:OP2    | 86:5:4109:OHX:N5   | 2.54                     | 0.41              |
| 36:5:3287:U:H2'    | 36:5:3288:G:C5'    | 2.51                     | 0.41              |
| 86:5:4125:OHX:N6   | 86:5:4200:OHX:N2   | 2.69                     | 0.41              |
| 37:7:55:A:HO2'     | 48:m1:152:HIS:HD1  | 1.67                     | 0.41              |
| 38:8:52:A:N6       | 75:o9:27:ILE:HD13  | 2.36                     | 0.41              |
| 40:l3:151:ILE:O    | 40:l3:155:ALA:HB3  | 2.21                     | 0.41              |
| 41:l4:23:PRO:O     | 41:l4:24:ALA:HB3   | 2.20                     | 0.41              |
| 41:l4:144:LYS:CG   | 41:l4:145:ILE:H    | 2.34                     | 0.41              |
| 42:l5:83:LEU:HB3   | 42:l5:88:ILE:HB    | 2.01                     | 0.41              |
| 47:m0:86:HIS:ND1   | 47:m0:139:ARG:NH1  | 2.57                     | 0.41              |
| 52:m6:126:VAL:HG23 | 52:m6:127:LEU:HD23 | 2.02                     | 0.41              |
| 54:m8:98:LYS:HB3   | 54:m8:99:THR:H     | 1.66                     | 0.41              |
| 54:m8:170:ARG:O    | 54:m8:170:ARG:HG3  | 2.20                     | 0.41              |
| 55:m9:7:GLN:HG2    | 55:m9:7:GLN:H      | 1.55                     | 0.41              |
| 63:n7:12:VAL:HB    | 63:n7:81:LEU:HB3   | 2.03                     | 0.41              |
| 68:o2:109:LEU:O    | 68:o2:110:ALA:C    | 2.63                     | 0.41              |
| 69:o3:6:ARG:HG3    | 69:o3:8:TYR:CE1    | 2.55                     | 0.41              |
| 1:2:237:C:C5'      | 1:2:238:U:H5'      | 2.40                     | 0.41              |
| 1:2:372:G:H1'      | 1:2:612:U:O2       | 2.21                     | 0.41              |
| 1:2:832:U:H2'      | 1:2:833:U:H5''     | 2.03                     | 0.41              |
| 2:S0:202:TYR:H     | 2:S0:202:TYR:HD2   | 1.69                     | 0.41              |
| 3:S1:72:ASP:OD2    | 28:D6:59:TYR:OH    | 2.24                     | 0.41              |
| 5:S3:207:THR:HB    | 19:C7:40:THR:OG1   | 2.20                     | 0.41              |
| 8:S6:147:LEU:O     | 8:S6:148:SER:OG    | 2.30                     | 0.41              |
| 9:S7:77:LEU:HD22   | 9:S7:81:LEU:HD11   | 2.03                     | 0.41              |
| 11:S9:41:GLU:OE1   | 11:S9:126:ARG:NH2  | 2.54                     | 0.41              |
| 14:C2:41:LEU:HD23  | 14:C2:41:LEU:HA    | 1.75                     | 0.41              |
| 17:C5:128:HIS:O    | 17:C5:130:ARG:HG2  | 2.21                     | 0.41              |
| 24:D2:86:ILE:HG13  | 24:D2:87:GLU:H     | 1.83                     | 0.41              |
| 29:D7:61:THR:O     | 29:D7:62:ILE:HB    | 2.21                     | 0.41              |
| 36:1:16:A:H2'      | 36:1:17:G:O4'      | 2.20                     | 0.41              |
| 36:1:685:G:OP2     | 49:M3:35:ARG:NH1   | 2.51                     | 0.41              |
| 36:1:795:G:O6      | 86:1:3898:OHX:N3   | 2.54                     | 0.41              |
| 36:1:1720:U:C4     | 55:M9:124:TYR:CE2  | 3.08                     | 0.41              |
| 36:1:2514:U:C6     | 45:L8:68:ARG:HB3   | 2.56                     | 0.41              |
| 40:L3:4:ARG:O      | 40:L3:5:LYS:CB     | 2.68                     | 0.41              |
| 40:L3:27:ALA:HB3   | 40:L3:218:ILE:HG22 | 2.01                     | 0.41              |
| 41:L4:52:VAL:CG1   | 41:L4:99:MET:HE3   | 2.51                     | 0.41              |
| 51:M5:173:GLY:HA3  | 51:M5:183:THR:OG1  | 2.20                     | 0.41              |
| 59:N3:48:ARG:HH11  | 59:N3:48:ARG:HG3   | 1.86                     | 0.41              |
| 60:N4:14:TYR:O     | 60:N4:17:ARG:HB3   | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:O4:67:LYS:O     | 70:O4:67:LYS:HG3   | 2.20                     | 0.41              |
| 1:6:220:A:OP2      | 1:6:832:U:H5''     | 2.21                     | 0.41              |
| 1:6:805:U:C2'      | 1:6:806:A:H5'      | 2.50                     | 0.41              |
| 1:6:817:A:H2'      | 1:6:818:C:C6       | 2.56                     | 0.41              |
| 1:6:1793:G:H4'     | 86:6:2126:OHX:N5   | 2.36                     | 0.41              |
| 4:s2:162:CYS:SG    | 4:s2:212:LYS:HE2   | 2.61                     | 0.41              |
| 6:s4:86:PHE:O      | 6:s4:87:MET:HB2    | 2.21                     | 0.41              |
| 7:s5:149:VAL:HG12  | 7:s5:156:ARG:O     | 2.21                     | 0.41              |
| 7:s5:189:THR:O     | 7:s5:193:THR:HG23  | 2.21                     | 0.41              |
| 9:s7:137:GLY:CA    | 9:s7:153:LEU:HB2   | 2.51                     | 0.41              |
| 10:s8:147:ALA:C    | 10:s8:149:SER:N    | 2.79                     | 0.41              |
| 11:s9:109:LEU:HB2  | 11:s9:146:PHE:HB3  | 2.02                     | 0.41              |
| 12:c0:70:GLU:O     | 12:c0:73:VAL:HG22  | 2.20                     | 0.41              |
| 16:c4:43:THR:OG1   | 16:c4:46:MET:HG3   | 2.20                     | 0.41              |
| 20:c8:89:GLN:HA    | 20:c8:97:ASP:HA    | 2.02                     | 0.41              |
| 23:d1:74:GLN:OE1   | 23:d1:82:VAL:N     | 2.54                     | 0.41              |
| 28:d6:33:ASP:C     | 28:d6:34:LYS:O     | 2.63                     | 0.41              |
| 30:d8:19:THR:HB    | 30:d8:20:GLY:H     | 1.65                     | 0.41              |
| 80:e0:46:ASN:OD1   | 80:e0:47:VAL:N     | 2.54                     | 0.41              |
| 36:5:357:A:O4'     | 41:l4:81:GLY:HA3   | 2.21                     | 0.41              |
| 36:5:618:C:H2'     | 36:5:619:A:C8      | 2.55                     | 0.41              |
| 36:5:726:G:H8      | 36:5:726:G:H5'     | 1.85                     | 0.41              |
| 36:5:748:U:H2'     | 36:5:749:C:C6      | 2.56                     | 0.41              |
| 36:5:874:U:H5''    | 36:5:2950:G:OP1    | 2.20                     | 0.41              |
| 36:5:1481:A:H2'    | 36:5:1858:A:N3     | 2.35                     | 0.41              |
| 36:5:1570:U:O2'    | 36:5:1571:A:O4'    | 2.37                     | 0.41              |
| 36:5:1639:C:C5'    | 70:o4:52:GLN:HG2   | 2.50                     | 0.41              |
| 36:5:1797:A:H2'    | 36:5:1798:A:O4'    | 2.21                     | 0.41              |
| 36:5:3242:G:N2     | 36:5:3245:A:H5''   | 2.35                     | 0.41              |
| 37:7:49:G:H4'      | 37:7:50:U:O5'      | 2.21                     | 0.41              |
| 37:7:64:A:C2       | 47:m0:202:LYS:HD3  | 2.55                     | 0.41              |
| 38:8:23:U:P        | 62:n6:16:ARG:HH21  | 2.44                     | 0.41              |
| 38:8:135:G:OP1     | 61:n5:49:LYS:HE3   | 2.21                     | 0.41              |
| 39:l2:242:ARG:HH11 | 39:l2:242:ARG:HG3  | 1.85                     | 0.41              |
| 40:l3:36:ASP:O     | 40:l3:38:SER:N     | 2.53                     | 0.41              |
| 40:l3:106:TRP:CH2  | 40:l3:161:LEU:HD13 | 2.55                     | 0.41              |
| 40:l3:139:GLN:HB2  | 40:l3:141:GLY:N    | 2.27                     | 0.41              |
| 40:l3:222:LYS:HG2  | 40:l3:223:GLY:N    | 2.35                     | 0.41              |
| 43:l6:56:LYS:HD2   | 43:l6:98:VAL:HG13  | 2.03                     | 0.41              |
| 47:m0:210:ILE:HG12 | 47:m0:217:PHE:CD2  | 2.56                     | 0.41              |
| 48:m1:151:SER:C    | 48:m1:152:HIS:O    | 2.63                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:m4:62:GLN:H     | 50:m4:62:GLN:HG2   | 1.66                     | 0.41              |
| 64:n8:70:LYS:HB2   | 64:n8:70:LYS:HE3   | 1.94                     | 0.41              |
| 66:o0:54:SER:OG    | 70:o4:94:LEU:HD13  | 2.20                     | 0.41              |
| 66:o0:81:VAL:HG11  | 66:o0:90:VAL:HG21  | 2.02                     | 0.41              |
| 69:o3:103:TYR:HA   | 69:o3:104:PRO:C    | 2.46                     | 0.41              |
| 74:o8:61:LYS:H     | 74:o8:61:LYS:HG2   | 1.27                     | 0.41              |
| 1:2:275:C:N3       | 1:2:276:C:N4       | 2.67                     | 0.41              |
| 1:2:552:G:C6       | 1:2:553:G:C6       | 3.09                     | 0.41              |
| 1:2:1116:A:P       | 77:Q1:17:ARG:HH21  | 2.44                     | 0.41              |
| 1:2:1220:C:H5''    | 12:C0:52:LYS:HD2   | 2.03                     | 0.41              |
| 1:2:1657:U:C5      | 36:1:2125:A:O3'    | 2.74                     | 0.41              |
| 3:S1:103:MET:HG2   | 3:S1:104:ASP:N     | 2.36                     | 0.41              |
| 4:S2:90:THR:C      | 4:S2:92:ALA:H      | 2.28                     | 0.41              |
| 6:S4:159:THR:HB    | 6:S4:227:VAL:HG23  | 2.03                     | 0.41              |
| 7:S5:205:SER:O     | 7:S5:207:THR:N     | 2.54                     | 0.41              |
| 9:S7:41:LEU:HD13   | 9:S7:70:PHE:HD1    | 1.85                     | 0.41              |
| 15:C3:114:ARG:HG2  | 15:C3:114:ARG:NH1  | 2.36                     | 0.41              |
| 19:C7:87:GLU:O     | 19:C7:88:VAL:HG12  | 2.20                     | 0.41              |
| 21:C9:42:GLY:CA    | 21:C9:84:LYS:HB2   | 2.49                     | 0.41              |
| 25:D3:42:PRO:O     | 25:D3:79:ASN:ND2   | 2.53                     | 0.41              |
| 28:D6:23:CYS:SG    | 28:D6:74:CYS:HB3   | 2.60                     | 0.41              |
| 28:D6:74:CYS:O     | 28:D6:75:VAL:HB    | 2.21                     | 0.41              |
| 34:SR:198:ASN:O    | 34:SR:215:GLY:HA3  | 2.21                     | 0.41              |
| 36:1:841:A:OP2     | 86:1:4178:OHX:N2   | 2.54                     | 0.41              |
| 36:1:1051:U:H4'    | 57:N1:19:PHE:CD2   | 2.55                     | 0.41              |
| 36:1:1262:G:C6     | 36:1:1278:A:N6     | 2.89                     | 0.41              |
| 36:1:1355:A:H1'    | 36:1:1356:U:OP2    | 2.21                     | 0.41              |
| 36:1:1486:G:N2     | 70:O4:6:THR:HG22   | 2.35                     | 0.41              |
| 36:1:1576:G:C6     | 36:1:1577:G:C2     | 3.09                     | 0.41              |
| 36:1:2597:U:H2'    | 36:1:2598:G:H8     | 1.86                     | 0.41              |
| 37:3:28:C:H6       | 37:3:28:C:O5'      | 2.03                     | 0.41              |
| 40:L3:308:MET:HE3  | 40:L3:308:MET:HB3  | 1.94                     | 0.41              |
| 41:L4:141:ARG:HH11 | 41:L4:141:ARG:HD3  | 1.67                     | 0.41              |
| 46:L9:141:LYS:HE2  | 46:L9:142:ASP:OD1  | 2.20                     | 0.41              |
| 47:M0:23:ASN:HB3   | 47:M0:24:ARG:H     | 1.70                     | 0.41              |
| 47:M0:99:ILE:HG13  | 47:M0:100:ASN:N    | 2.32                     | 0.41              |
| 53:M7:30:ARG:C     | 53:M7:30:ARG:HD3   | 2.46                     | 0.41              |
| 54:M8:102:ALA:CB   | 54:M8:122:ILE:HG22 | 2.51                     | 0.41              |
| 59:N3:130:ALA:O    | 59:N3:131:SER:C    | 2.63                     | 0.41              |
| 69:O3:60:ARG:HB2   | 69:O3:60:ARG:CZ    | 2.49                     | 0.41              |
| 72:O6:27:SER:O     | 72:O6:28:TYR:CB    | 2.67                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:336:G:H5'      | 13:c1:130:PRO:O    | 2.21                     | 0.41              |
| 1:6:578:U:O2       | 86:6:2154:OHX:N3   | 2.54                     | 0.41              |
| 1:6:586:G:H4'      | 80:e0:21:VAL:HG22  | 2.03                     | 0.41              |
| 1:6:951:A:O2'      | 15:c3:98:VAL:HG22  | 2.21                     | 0.41              |
| 3:s1:74:GLN:NE2    | 3:s1:189:ILE:HG21  | 2.36                     | 0.41              |
| 4:s2:54:GLU:H      | 4:s2:54:GLU:HG2    | 1.39                     | 0.41              |
| 5:s3:40:ARG:HE     | 22:d0:110:PRO:HG3  | 1.85                     | 0.41              |
| 14:c2:40:GLY:O     | 14:c2:124:LYS:N    | 2.39                     | 0.41              |
| 14:c2:46:ARG:HG2   | 14:c2:50:LYS:HD3   | 2.03                     | 0.41              |
| 16:c4:13:VAL:HG23  | 16:c4:76:ILE:HA    | 2.03                     | 0.41              |
| 16:c4:121:VAL:HA   | 16:c4:122:PRO:HD3  | 1.95                     | 0.41              |
| 31:d9:6:VAL:HG23   | 31:d9:7:TRP:CE3    | 2.56                     | 0.41              |
| 33:e1:119:ARG:O    | 33:e1:132:LEU:HG   | 2.21                     | 0.41              |
| 36:5:687:U:O2'     | 36:5:688:G:H5'     | 2.20                     | 0.41              |
| 36:5:873:C:H3'     | 36:5:874:U:H4'     | 2.01                     | 0.41              |
| 36:5:1340:G:OP2    | 68:o2:61:LYS:HD2   | 2.21                     | 0.41              |
| 36:5:1447:G:OP2    | 53:m7:27:LYS:NZ    | 2.40                     | 0.41              |
| 36:5:1639:C:N4     | 63:n7:17:ARG:HG3   | 2.36                     | 0.41              |
| 36:5:2213:A:H2'    | 36:5:2214:A:C8     | 2.56                     | 0.41              |
| 36:5:2217:U:H2'    | 36:5:2218:G:C8     | 2.56                     | 0.41              |
| 36:5:2286:U:C4     | 36:5:2288:G:H1'    | 2.56                     | 0.41              |
| 36:5:2360:C:H5''   | 36:5:2361:A:P      | 2.61                     | 0.41              |
| 36:5:3288:G:O2'    | 36:5:3289:G:H8     | 2.03                     | 0.41              |
| 38:8:149:A:H2'     | 38:8:150:G:C8      | 2.55                     | 0.41              |
| 41:l4:222:VAL:HG22 | 41:l4:225:VAL:HG23 | 2.02                     | 0.41              |
| 44:l7:96:PRO:HA    | 44:l7:97:PRO:HD3   | 1.83                     | 0.41              |
| 46:l9:114:VAL:HB   | 46:l9:124:ARG:HB2  | 2.02                     | 0.41              |
| 46:l9:120:ASP:OD1  | 46:l9:124:ARG:NH2  | 2.54                     | 0.41              |
| 47:m0:48:LEU:HD22  | 47:m0:49:CYS:N     | 2.36                     | 0.41              |
| 47:m0:208:ASN:O    | 47:m0:212:GLU:HB2  | 2.21                     | 0.41              |
| 51:m5:143:ARG:NH2  | 71:o5:92:LEU:HD23  | 2.35                     | 0.41              |
| 62:n6:45:ILE:HD12  | 62:n6:119:ILE:HG23 | 2.02                     | 0.41              |
| 68:o2:19:ARG:HD2   | 68:o2:28:VAL:HG13  | 2.02                     | 0.41              |
| 71:o5:21:LEU:CD2   | 71:o5:25:LYS:HE3   | 2.51                     | 0.41              |
| 1:2:196:G:HO2'     | 1:2:197:A:P        | 2.42                     | 0.41              |
| 1:2:491:C:H42      | 1:2:496:G:H1       | 1.68                     | 0.41              |
| 1:2:525:A:C6       | 1:2:526:A:C6       | 3.08                     | 0.41              |
| 1:2:639:U:P        | 9:S7:117:THR:HG1   | 2.41                     | 0.41              |
| 1:2:683:C:H2'      | 1:2:684:A:C8       | 2.56                     | 0.41              |
| 1:2:763:G:C6       | 1:2:764:U:C4       | 3.09                     | 0.41              |
| 1:2:819:G:O6       | 1:2:853:G:C5       | 2.74                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2:1170:G:C2      | 1:2:1171:A:C8     | 3.09                     | 0.41              |
| 1:2:1274:C:N4      | 35:SM:95:SER:HA   | 2.36                     | 0.41              |
| 1:2:1340:U:C2      | 1:2:1378:U:H4'    | 2.55                     | 0.41              |
| 1:2:1402:G:H2'     | 1:2:1403:C:C6     | 2.56                     | 0.41              |
| 1:2:1546:G:H21     | 20:C8:87:ASN:HB2  | 1.86                     | 0.41              |
| 1:2:1602:C:H2'     | 1:2:1603:U:O4'    | 2.21                     | 0.41              |
| 1:2:1623:C:H2'     | 1:2:1624:C:C6     | 2.56                     | 0.41              |
| 1:2:1759:C:H5''    | 1:2:1760:G:OP2    | 2.21                     | 0.41              |
| 86:2:2084:OHX:N4   | 86:2:2086:OHX:N1  | 2.69                     | 0.41              |
| 2:S0:110:TYR:HA    | 2:S0:115:PHE:CE1  | 2.56                     | 0.41              |
| 2:S0:167:LYS:HD3   | 2:S0:168:HIS:CD2  | 2.56                     | 0.41              |
| 3:S1:184:LEU:HA    | 3:S1:187:LYS:HB2  | 2.03                     | 0.41              |
| 4:S2:59:HIS:CD2    | 4:S2:238:SER:HA   | 2.55                     | 0.41              |
| 5:S3:25:PHE:HE1    | 5:S3:69:LEU:HD22  | 1.86                     | 0.41              |
| 6:S4:158:ASP:OD1   | 6:S4:158:ASP:N    | 2.52                     | 0.41              |
| 6:S4:193:GLY:C     | 6:S4:194:THR:HG1  | 2.28                     | 0.41              |
| 7:S5:35:GLN:HB3    | 7:S5:36:ALA:H     | 1.59                     | 0.41              |
| 7:S5:36:ALA:HB3    | 7:S5:45:LYS:NZ    | 2.36                     | 0.41              |
| 8:S6:214:LYS:HA    | 8:S6:217:SER:OG   | 2.21                     | 0.41              |
| 10:S8:9:HIS:O      | 10:S8:10:LYS:CB   | 2.68                     | 0.41              |
| 11:S9:133:HIS:CD2  | 11:S9:162:SER:HB2 | 2.56                     | 0.41              |
| 11:S9:138:LYS:HE2  | 26:D4:67:GLY:HA3  | 2.03                     | 0.41              |
| 14:C2:45:LEU:O     | 14:C2:49:THR:HG23 | 2.21                     | 0.41              |
| 15:C3:52:VAL:HG22  | 15:C3:55:ARG:NH2  | 2.36                     | 0.41              |
| 20:C8:26:ILE:HG13  | 20:C8:27:LYS:N    | 2.31                     | 0.41              |
| 24:D2:86:ILE:HD11  | 24:D2:117:ARG:HD3 | 2.02                     | 0.41              |
| 27:D5:39:ALA:O     | 27:D5:71:ILE:HA   | 2.21                     | 0.41              |
| 34:SR:7:LEU:H      | 34:SR:7:LEU:HD12  | 1.86                     | 0.41              |
| 34:SR:52:GLN:H     | 34:SR:52:GLN:CD   | 2.29                     | 0.41              |
| 34:SR:167:VAL:HG12 | 34:SR:183:LEU:HB2 | 2.03                     | 0.41              |
| 34:SR:275:ARG:HA   | 34:SR:276:PRO:HD2 | 1.96                     | 0.41              |
| 36:1:520:U:N3      | 41:L4:347:THR:O   | 2.54                     | 0.41              |
| 36:1:789:A:H2'     | 36:1:790:U:H6     | 1.85                     | 0.41              |
| 36:1:1015:U:O2'    | 36:1:1017:C:OP2   | 2.31                     | 0.41              |
| 36:1:1081:U:OP2    | 36:1:1081:U:H4'   | 2.21                     | 0.41              |
| 36:1:1194:G:OP1    | 86:1:3967:OHX:N1  | 2.54                     | 0.41              |
| 36:1:1285:G:O2'    | 36:1:1286:A:OP2   | 2.30                     | 0.41              |
| 36:1:1424:C:H2'    | 36:1:1425:U:O4'   | 2.21                     | 0.41              |
| 36:1:1844:C:O2     | 73:O7:9:GLY:HA2   | 2.20                     | 0.41              |
| 36:1:1927:G:P      | 79:Q3:6:LYS:H     | 2.43                     | 0.41              |
| 36:1:2138:A:C4     | 73:O7:3:LYS:HB3   | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:1:2158:A:O4'   | 36:1:2160:G:C8     | 2.74                     | 0.41              |
| 36:1:2536:A:H2'   | 36:1:2537:U:C5     | 2.55                     | 0.41              |
| 36:1:2635:A:H4'   | 36:1:2636:A:O5'    | 2.21                     | 0.41              |
| 36:1:2842:U:OP1   | 36:1:2844:C:N4     | 2.53                     | 0.41              |
| 36:1:3251:U:H2'   | 36:1:3252:G:C8     | 2.56                     | 0.41              |
| 38:4:85:G:H3'     | 38:4:85:G:H8       | 1.86                     | 0.41              |
| 40:L3:49:TYR:O    | 40:L3:80:ASP:N     | 2.53                     | 0.41              |
| 40:L3:76:VAL:HG11 | 40:L3:323:MET:HE3  | 2.03                     | 0.41              |
| 40:L3:83:PRO:O    | 40:L3:165:GLN:HG3  | 2.21                     | 0.41              |
| 40:L3:265:ALA:C   | 40:L3:266:ARG:HG2  | 2.46                     | 0.41              |
| 41:L4:291:ASN:O   | 41:L4:292:SER:C    | 2.62                     | 0.41              |
| 41:L4:316:ASN:C   | 41:L4:317:PRO:O    | 2.64                     | 0.41              |
| 46:L9:129:ARG:O   | 46:L9:132:VAL:HG13 | 2.21                     | 0.41              |
| 49:M3:64:LYS:HG3  | 64:N8:69:TRP:CD2   | 2.56                     | 0.41              |
| 50:M4:108:ARG:HA  | 50:M4:108:ARG:HD2  | 1.94                     | 0.41              |
| 51:M5:73:ARG:NH1  | 51:M5:88:GLY:O     | 2.47                     | 0.41              |
| 54:M8:64:VAL:HG11 | 54:M8:113:LYS:HD2  | 2.02                     | 0.41              |
| 55:M9:106:LEU:HB3 | 55:M9:120:TYR:CE1  | 2.55                     | 0.41              |
| 58:N2:90:ARG:O    | 58:N2:91:ASP:HB2   | 2.20                     | 0.41              |
| 62:N6:53:ASP:HB2  | 62:N6:110:HIS:CD2  | 2.56                     | 0.41              |
| 63:N7:97:SER:O    | 63:N7:100:THR:HB   | 2.21                     | 0.41              |
| 67:O1:46:THR:HG21 | 67:O1:91:SER:OG    | 2.21                     | 0.41              |
| 72:O6:95:ALA:O    | 72:O6:96:ALA:C     | 2.63                     | 0.41              |
| 1:6:325:G:C2      | 1:6:344:A:C2       | 3.09                     | 0.41              |
| 1:6:491:C:H42     | 1:6:497:G:H21      | 1.69                     | 0.41              |
| 1:6:682:C:H2'     | 1:6:683:C:C6       | 2.56                     | 0.41              |
| 1:6:832:U:OP2     | 86:6:2202:OHX:N6   | 2.54                     | 0.41              |
| 1:6:1198:G:O3'    | 31:d9:40:ARG:NH2   | 2.53                     | 0.41              |
| 1:6:1357:A:H2'    | 1:6:1358:G:C8      | 2.55                     | 0.41              |
| 1:6:1429:G:H21    | 22:d0:72:ASN:HD21  | 1.67                     | 0.41              |
| 1:6:1645:G:OP2    | 86:6:2183:OHX:N3   | 2.54                     | 0.41              |
| 1:6:1698:G:H1'    | 1:6:1699:G:OP1     | 2.20                     | 0.41              |
| 1:6:1756:A:H2'    | 1:6:1757:G:H8      | 1.86                     | 0.41              |
| 2:s0:37:VAL:HG22  | 2:s0:149:LEU:HD13  | 2.02                     | 0.41              |
| 5:s3:219:ALA:HA   | 5:s3:220:PRO:HD2   | 1.83                     | 0.41              |
| 9:s7:55:LYS:HE2   | 9:s7:87:ASP:HA     | 2.03                     | 0.41              |
| 9:s7:133:THR:HG22 | 9:s7:157:LYS:O     | 2.21                     | 0.41              |
| 10:s8:8:ARG:NH2   | 10:s8:22:ARG:HH11  | 2.11                     | 0.41              |
| 11:s9:117:GLY:C   | 11:s9:119:ALA:H    | 2.29                     | 0.41              |
| 13:c1:77:SER:HB3  | 13:c1:85:VAL:HB    | 2.02                     | 0.41              |
| 15:c3:48:SER:O    | 15:c3:52:VAL:HG23  | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:c4:33:LEU:HD13  | 16:c4:33:LEU:HA    | 1.87                     | 0.41              |
| 17:c5:77:ARG:HB3   | 17:c5:102:PHE:CD1  | 2.56                     | 0.41              |
| 20:c8:7:GLU:HB3    | 20:c8:10:SER:OG    | 2.20                     | 0.41              |
| 23:d1:85:TYR:CD1   | 29:d7:6:ASP:HB2    | 2.56                     | 0.41              |
| 27:d5:43:ASP:O     | 27:d5:44:GLN:HB3   | 2.21                     | 0.41              |
| 28:d6:66:LYS:HB2   | 28:d6:68:TYR:CE2   | 2.56                     | 0.41              |
| 35:sM:51:ARG:CZ    | 35:sM:52:PRO:HD2   | 2.50                     | 0.41              |
| 36:5:34:A:C4       | 36:5:51:A:C2       | 3.09                     | 0.41              |
| 36:5:269:G:H5'     | 51:m5:120:TRP:CE3  | 2.56                     | 0.41              |
| 36:5:271:C:H2'     | 36:5:272:G:O4'     | 2.21                     | 0.41              |
| 36:5:277:G:H2'     | 36:5:278:U:C6      | 2.56                     | 0.41              |
| 36:5:278:U:O5'     | 36:5:278:U:H6      | 2.04                     | 0.41              |
| 36:5:279:U:H2'     | 36:5:280:U:H6      | 1.86                     | 0.41              |
| 36:5:611:A:O4'     | 43:l6:23:LYS:HE3   | 2.21                     | 0.41              |
| 36:5:904:A:H2      | 39:l2:15:ILE:HD11  | 1.84                     | 0.41              |
| 36:5:1012:G:H2'    | 36:5:1013:G:O4'    | 2.21                     | 0.41              |
| 36:5:1080:A:OP1    | 42:l5:140:ARG:HD3  | 2.21                     | 0.41              |
| 36:5:1632:A:H2'    | 36:5:1633:C:C6     | 2.56                     | 0.41              |
| 36:5:1713:G:O6     | 66:o0:28:LYS:HD3   | 2.20                     | 0.41              |
| 36:5:1716:U:H3'    | 36:5:1716:U:P      | 2.61                     | 0.41              |
| 36:5:2101:C:O2'    | 36:5:2102:U:P      | 2.78                     | 0.41              |
| 36:5:2162:U:P      | 39:l2:227:ARG:HH21 | 2.43                     | 0.41              |
| 36:5:2549:G:C2     | 45:l8:33:ASN:ND2   | 2.89                     | 0.41              |
| 36:5:2552:C:H5     | 66:o0:53:LYS:NZ    | 2.19                     | 0.41              |
| 36:5:3078:U:H4'    | 36:5:3079:U:O5'    | 2.21                     | 0.41              |
| 36:5:3136:G:OP2    | 86:5:4106:OHX:N3   | 2.54                     | 0.41              |
| 36:5:3284:G:OP2    | 36:5:3284:G:H8     | 2.03                     | 0.41              |
| 86:5:4177:OHX:N4   | 86:5:4238:OHX:N1   | 2.69                     | 0.41              |
| 39:l2:92:LYS:HA    | 39:l2:103:PRO:CD   | 2.51                     | 0.41              |
| 39:l2:112:ILE:HD11 | 79:q3:79:VAL:HG11  | 2.03                     | 0.41              |
| 39:l2:217:GLN:O    | 39:l2:218:HIS:HB3  | 2.20                     | 0.41              |
| 43:l6:55:LEU:HD12  | 43:l6:64:LEU:HD13  | 2.02                     | 0.41              |
| 44:l7:121:LYS:HB2  | 57:n1:133:ALA:HB3  | 2.02                     | 0.41              |
| 44:l7:175:LYS:HD3  | 44:l7:176:TYR:CZ   | 2.55                     | 0.41              |
| 47:m0:175:ASN:CG   | 47:m0:176:LEU:N    | 2.74                     | 0.41              |
| 49:m3:3:ILE:HG12   | 64:n8:34:MET:CE    | 2.51                     | 0.41              |
| 50:m4:32:LEU:HD11  | 50:m4:94:TRP:CG    | 2.56                     | 0.41              |
| 51:m5:101:THR:O    | 51:m5:105:ARG:HG2  | 2.21                     | 0.41              |
| 57:n1:88:ARG:H     | 57:n1:88:ARG:HG2   | 1.77                     | 0.41              |
| 59:n3:69:LEU:HD12  | 59:n3:69:LEU:HA    | 1.82                     | 0.41              |
| 60:n4:52:THR:O     | 60:n4:56:ARG:HG3   | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:n5:115:ARG:NH1 | 61:n5:119:THR:OG1  | 2.53                     | 0.41              |
| 62:n6:115:ARG:HG3 | 62:n6:115:ARG:NH1  | 2.35                     | 0.41              |
| 62:n6:120:GLN:CD  | 62:n6:126:LEU:HA   | 2.45                     | 0.41              |
| 64:n8:43:ILE:O    | 64:n8:46:ASP:O     | 2.39                     | 0.41              |
| 64:n8:65:GLN:OE1  | 64:n8:65:GLN:HA    | 2.20                     | 0.41              |
| 70:o4:74:ARG:HD3  | 70:o4:85:VAL:HG21  | 2.02                     | 0.41              |
| 70:o4:103:LYS:HA  | 70:o4:103:LYS:HD3  | 1.95                     | 0.41              |
| 82:p0:37:GLN:O    | 82:p0:41:VAL:HG23  | 2.20                     | 0.41              |
| 82:p0:188:VAL:O   | 82:p0:189:GLN:HG2  | 2.21                     | 0.41              |
| 1:2:71:A:H2'      | 1:2:72:A:O4'       | 2.20                     | 0.41              |
| 1:2:88:U:H4'      | 1:2:171:A:O4'      | 2.21                     | 0.41              |
| 1:2:199:G:O2'     | 1:2:200:A:H8       | 2.04                     | 0.41              |
| 1:2:288:A:H2'     | 1:2:289:U:O4'      | 2.20                     | 0.41              |
| 1:2:512:A:HO2'    | 1:2:513:U:P        | 2.44                     | 0.41              |
| 1:2:639:U:H4'     | 1:2:639:U:OP2      | 2.21                     | 0.41              |
| 1:2:964:U:H5''    | 15:C3:128:TYR:CE1  | 2.56                     | 0.41              |
| 1:2:1433:G:N2     | 31:D9:45:GLU:OE1   | 2.51                     | 0.41              |
| 1:2:1636:C:C2     | 1:2:1638:G:C5      | 3.09                     | 0.41              |
| 1:2:1793:G:O2'    | 28:D6:5:ARG:NH2    | 2.54                     | 0.41              |
| 3:S1:101:HIS:HA   | 3:S1:217:LEU:HD22  | 2.03                     | 0.41              |
| 5:S3:137:VAL:HG22 | 5:S3:151:LYS:HG3   | 2.01                     | 0.41              |
| 5:S3:194:LYS:O    | 5:S3:196:ARG:N     | 2.54                     | 0.41              |
| 6:S4:180:LEU:HD23 | 6:S4:180:LEU:HA    | 1.74                     | 0.41              |
| 10:S8:76:THR:HB   | 10:S8:105:ASP:CB   | 2.51                     | 0.41              |
| 11:S9:37:LYS:HB3  | 32:E0:33:ARG:HB2   | 2.03                     | 0.41              |
| 16:C4:30:VAL:HG13 | 16:C4:39:ILE:O     | 2.21                     | 0.41              |
| 18:C6:123:ARG:HE  | 18:C6:123:ARG:HB2  | 1.51                     | 0.41              |
| 24:D2:77:PRO:HD2  | 24:D2:79:PHE:CE2   | 2.56                     | 0.41              |
| 28:D6:38:ARG:HH21 | 28:D6:83:ILE:CG1   | 2.33                     | 0.41              |
| 33:E1:82:LYS:HB3  | 33:E1:82:LYS:HE2   | 1.82                     | 0.41              |
| 36:1:916:G:H1     | 39:L2:207:VAL:HG11 | 1.85                     | 0.41              |
| 36:1:1571:A:H2'   | 36:1:1572:U:O4'    | 2.20                     | 0.41              |
| 36:1:1610:G:H2'   | 36:1:1611:G:O4'    | 2.20                     | 0.41              |
| 36:1:2369:G:H2'   | 36:1:2370:G:C8     | 2.56                     | 0.41              |
| 36:1:3343:G:N2    | 36:1:3362:A:H2     | 1.93                     | 0.41              |
| 86:1:4088:OHX:N2  | 86:1:4157:OHX:N1   | 2.69                     | 0.41              |
| 38:4:1:A:H2'      | 38:4:2:A:O5'       | 2.21                     | 0.41              |
| 41:L4:205:PRO:HB3 | 41:L4:247:PHE:CD2  | 2.56                     | 0.41              |
| 42:L5:258:LYS:O   | 42:L5:259:LYS:HG2  | 2.21                     | 0.41              |
| 45:L8:70:LYS:HD2  | 45:L8:70:LYS:HA    | 1.90                     | 0.41              |
| 46:L9:116:ASN:O   | 46:L9:119:GLY:N    | 2.53                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:M4:8:LYS:O      | 50:M4:9:ALA:HB2   | 2.21                     | 0.41              |
| 51:M5:183:THR:HA   | 51:M5:187:ARG:HB2 | 2.03                     | 0.41              |
| 52:M6:186:ALA:C    | 52:M6:188:SER:H   | 2.29                     | 0.41              |
| 54:M8:19:PRO:HB3   | 54:M8:53:PHE:HA   | 2.02                     | 0.41              |
| 55:M9:21:LYS:HE3   | 55:M9:55:VAL:HA   | 2.03                     | 0.41              |
| 56:N0:1:MET:HE3    | 56:N0:2:ALA:HB3   | 2.03                     | 0.41              |
| 57:N1:41:ASP:OD1   | 57:N1:99:SER:HB2  | 2.21                     | 0.41              |
| 57:N1:120:LYS:HE3  | 57:N1:120:LYS:HB2 | 1.92                     | 0.41              |
| 59:N3:48:ARG:HG3   | 59:N3:48:ARG:NH1  | 2.36                     | 0.41              |
| 63:N7:47:GLU:OE2   | 63:N7:69:LYS:HE2  | 2.21                     | 0.41              |
| 64:N8:7:LYS:HD3    | 64:N8:7:LYS:HA    | 1.79                     | 0.41              |
| 65:N9:17:HIS:O     | 86:N9:101:OHX:N6  | 2.53                     | 0.41              |
| 67:O1:72:ARG:O     | 67:O1:96:VAL:HG13 | 2.21                     | 0.41              |
| 67:O1:79:ARG:H     | 67:O1:79:ARG:HE   | 1.69                     | 0.41              |
| 69:O3:49:ILE:HD11  | 69:O3:70:LYS:C    | 2.46                     | 0.41              |
| 70:O4:8:ARG:NH1    | 70:O4:8:ARG:HG2   | 2.36                     | 0.41              |
| 70:O4:74:ARG:NH2   | 70:O4:82:ALA:HB2  | 2.36                     | 0.41              |
| 72:O6:95:ALA:O     | 72:O6:99:ARG:HB2  | 2.20                     | 0.41              |
| 1:6:523:G:O2'      | 1:6:529:A:N6      | 2.50                     | 0.41              |
| 1:6:703:G:H2'      | 1:6:704:C:C6      | 2.56                     | 0.41              |
| 1:6:1130:G:OP2     | 86:6:2113:OHX:N1  | 2.54                     | 0.41              |
| 1:6:1180:C:O2'     | 17:c5:128:HIS:HA  | 2.21                     | 0.41              |
| 1:6:1359:C:O5'     | 1:6:1359:C:H6     | 2.04                     | 0.41              |
| 1:6:1395:G:O6      | 86:6:2089:OHX:N3  | 2.54                     | 0.41              |
| 1:6:1504:G:OP1     | 21:c9:97:SER:OG   | 2.34                     | 0.41              |
| 86:6:2150:OHX:N1   | 86:c1:202:OHX:N2  | 2.69                     | 0.41              |
| 3:s1:120:LEU:CD2   | 3:s1:122:GLU:HG3  | 2.50                     | 0.41              |
| 6:s4:43:PRO:HA     | 6:s4:82:TYR:O     | 2.21                     | 0.41              |
| 6:s4:50:ASN:O      | 6:s4:53:LYS:NZ    | 2.54                     | 0.41              |
| 7:s5:73:THR:CG2    | 18:c6:114:ARG:HE  | 2.34                     | 0.41              |
| 9:s7:55:LYS:HE2    | 9:s7:55:LYS:HB3   | 1.83                     | 0.41              |
| 12:c0:23:ALA:CB    | 12:c0:64:TYR:HB2  | 2.51                     | 0.41              |
| 15:c3:16:ILE:HD12  | 15:c3:16:ILE:HA   | 1.75                     | 0.41              |
| 15:c3:47:PRO:HG2   | 15:c3:72:MET:HG3  | 2.02                     | 0.41              |
| 16:c4:16:VAL:O     | 16:c4:30:VAL:HA   | 2.21                     | 0.41              |
| 16:c4:110:LEU:HD23 | 16:c4:110:LEU:HA  | 1.94                     | 0.41              |
| 17:c5:126:VAL:HG22 | 17:c5:127:ARG:N   | 2.36                     | 0.41              |
| 19:c7:44:LYS:HG3   | 19:c7:47:ARG:NH1  | 2.35                     | 0.41              |
| 20:c8:61:LEU:HA    | 20:c8:65:GLU:OE1  | 2.21                     | 0.41              |
| 24:d2:38:LEU:HD23  | 24:d2:41:MET:CE   | 2.51                     | 0.41              |
| 24:d2:103:ILE:HD13 | 24:d2:126:LEU:HB2 | 2.03                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:d7:33:LEU:HD13 | 29:d7:73:LEU:HD21  | 2.02                     | 0.41              |
| 34:sR:255:ALA:N   | 34:sR:292:LEU:HD11 | 2.35                     | 0.41              |
| 36:5:2358:A:H2'   | 36:5:2359:C:O4'    | 2.20                     | 0.41              |
| 36:5:2770:G:H2'   | 36:5:2771:U:H5'    | 2.03                     | 0.41              |
| 36:5:2924:U:O4    | 86:5:4059:OHX:N2   | 2.54                     | 0.41              |
| 36:5:3285:C:H3'   | 36:5:3286:G:H5''   | 2.02                     | 0.41              |
| 86:5:4076:OHX:N5  | 86:o4:203:OHX:N6   | 2.68                     | 0.41              |
| 86:5:4093:OHX:N3  | 86:5:4199:OHX:N1   | 2.69                     | 0.41              |
| 42:l5:143:LYS:HG3 | 42:l5:172:TYR:HD2  | 1.86                     | 0.41              |
| 42:l5:259:LYS:H   | 42:l5:259:LYS:HG2  | 1.42                     | 0.41              |
| 42:l5:268:GLU:C   | 42:l5:270:LYS:N    | 2.79                     | 0.41              |
| 46:l9:38:LEU:HA   | 46:l9:38:LEU:HD23  | 1.86                     | 0.41              |
| 48:m1:7:ASN:H     | 48:m1:8:PRO:HD3    | 1.86                     | 0.41              |
| 51:m5:73:ARG:HB2  | 51:m5:92:LEU:HD23  | 2.02                     | 0.41              |
| 56:n0:49:HIS:HB3  | 56:n0:51:VAL:HG23  | 2.02                     | 0.41              |
| 61:n5:105:VAL:CG1 | 61:n5:126:LEU:HD22 | 2.51                     | 0.41              |
| 68:o2:20:HIS:CG   | 68:o2:42:VAL:HG21  | 2.55                     | 0.41              |
| 74:o8:41:THR:HG21 | 74:o8:62:ALA:CB    | 2.51                     | 0.41              |
| 1:2:268:C:N4      | 8:S6:186:ARG:HD2   | 2.36                     | 0.40              |
| 1:2:685:A:O2'     | 1:2:686:C:H5'      | 2.21                     | 0.40              |
| 1:2:702:G:N2      | 1:2:703:G:H1'      | 2.36                     | 0.40              |
| 1:2:941:A:O2'     | 1:2:977:A:H5'      | 2.21                     | 0.40              |
| 1:2:1474:G:H2'    | 1:2:1475:A:C8      | 2.56                     | 0.40              |
| 2:S0:189:VAL:HG22 | 2:S0:190:ASP:H     | 1.85                     | 0.40              |
| 6:S4:233:LYS:H    | 6:S4:233:LYS:HD2   | 1.85                     | 0.40              |
| 9:S7:43:PHE:CE1   | 9:S7:46:ILE:HG13   | 2.57                     | 0.40              |
| 11:S9:49:LEU:HD23 | 11:S9:104:PHE:CE2  | 2.56                     | 0.40              |
| 16:C4:129:LYS:HB2 | 16:C4:129:LYS:HE3  | 1.84                     | 0.40              |
| 28:D6:38:ARG:O    | 28:D6:71:LEU:N     | 2.51                     | 0.40              |
| 34:SR:21:THR:O    | 34:SR:291:SER:HB3  | 2.21                     | 0.40              |
| 36:1:661:G:N7     | 64:N8:19:LYS:HE3   | 2.36                     | 0.40              |
| 36:1:979:U:H1'    | 36:1:980:A:N7      | 2.29                     | 0.40              |
| 36:1:1207:G:N7    | 86:1:4066:OHX:N2   | 2.70                     | 0.40              |
| 36:1:1307:G:C2    | 36:1:1308:A:C2     | 3.08                     | 0.40              |
| 36:1:1528:G:N3    | 36:1:1588:A:H2     | 2.19                     | 0.40              |
| 36:1:2328:U:H2'   | 36:1:2329:C:C6     | 2.56                     | 0.40              |
| 36:1:2333:C:H2'   | 36:1:2334:U:C1'    | 2.50                     | 0.40              |
| 36:1:2392:C:O2    | 36:1:2987:A:N1     | 2.54                     | 0.40              |
| 36:1:2554:A:H5''  | 39:L2:85:GLY:O     | 2.20                     | 0.40              |
| 36:1:2677:G:H2'   | 36:1:2679:A:H2     | 1.86                     | 0.40              |
| 41:L4:138:ARG:HG3 | 41:L4:244:LEU:O    | 2.21                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:L5:78:ALA:HB3   | 42:L5:105:ILE:HG12 | 2.03                     | 0.40              |
| 46:L9:86:TYR:CE1   | 46:L9:151:VAL:HG13 | 2.56                     | 0.40              |
| 47:M0:174:THR:HG23 | 47:M0:176:LEU:N    | 2.10                     | 0.40              |
| 49:M3:47:ALA:HB1   | 49:M3:48:PRO:CD    | 2.51                     | 0.40              |
| 49:M3:56:PRO:HG3   | 49:M3:74:GLY:O     | 2.22                     | 0.40              |
| 49:M3:135:ALA:O    | 49:M3:136:GLU:HB3  | 2.20                     | 0.40              |
| 51:M5:186:GLY:O    | 51:M5:190:THR:HG22 | 2.21                     | 0.40              |
| 52:M6:129:LEU:HD12 | 52:M6:129:LEU:HA   | 1.87                     | 0.40              |
| 53:M7:50:GLN:OE1   | 53:M7:56:ARG:HD3   | 2.21                     | 0.40              |
| 55:M9:168:ALA:O    | 55:M9:172:ARG:HD2  | 2.21                     | 0.40              |
| 61:N5:79:GLY:O     | 61:N5:81:ILE:HG13  | 2.20                     | 0.40              |
| 64:N8:2:PRO:HG2    | 64:N8:5:PHE:CD2    | 2.56                     | 0.40              |
| 72:O6:98:ARG:HD2   | 72:O6:98:ARG:H     | 1.86                     | 0.40              |
| 77:Q1:16:LYS:O     | 77:Q1:20:VAL:HG23  | 2.21                     | 0.40              |
| 1:6:90:C:O2'       | 1:6:91:G:H5'       | 2.21                     | 0.40              |
| 1:6:329:G:H2'      | 1:6:330:G:C8       | 2.56                     | 0.40              |
| 1:6:615:A:N3       | 1:6:1107:G:C2      | 2.89                     | 0.40              |
| 1:6:958:U:H5'      | 29:d7:49:HIS:CD2   | 2.56                     | 0.40              |
| 1:6:1253:U:H4'     | 33:e1:143:LYS:CA   | 2.51                     | 0.40              |
| 1:6:1281:G:C2      | 1:6:1282:U:C2      | 3.09                     | 0.40              |
| 86:6:2128:OHX:N5   | 86:d9:102:OHX:N3   | 2.69                     | 0.40              |
| 3:s1:104:ASP:CG    | 3:s1:214:LYS:HE2   | 2.46                     | 0.40              |
| 5:s3:90:ARG:HB3    | 5:s3:91:VAL:H      | 1.59                     | 0.40              |
| 6:s4:38:LEU:C      | 6:s4:38:LEU:HD12   | 2.45                     | 0.40              |
| 6:s4:62:LYS:HZ1    | 6:s4:66:MET:HE3    | 1.85                     | 0.40              |
| 6:s4:105:VAL:HG13  | 6:s4:243:GLY:HA2   | 2.03                     | 0.40              |
| 8:s6:122:GLU:C     | 8:s6:124:LEU:H     | 2.28                     | 0.40              |
| 11:s9:28:LEU:HD11  | 80:e0:39:LEU:HB3   | 2.03                     | 0.40              |
| 11:s9:48:GLN:O     | 11:s9:52:ILE:HG13  | 2.20                     | 0.40              |
| 14:c2:25:GLU:C     | 14:c2:27:ALA:H     | 2.28                     | 0.40              |
| 17:c5:35:LYS:HE2   | 17:c5:35:LYS:HB3   | 1.89                     | 0.40              |
| 33:e1:80:ARG:HB2   | 33:e1:80:ARG:HH11  | 1.85                     | 0.40              |
| 36:5:428:A:H2'     | 36:5:429:U:C6      | 2.56                     | 0.40              |
| 36:5:879:U:O2      | 36:5:2357:A:H1'    | 2.21                     | 0.40              |
| 36:5:1025:A:H5'    | 36:5:1026:A:OP2    | 2.20                     | 0.40              |
| 36:5:1027:A:N7     | 36:5:1029:G:C2     | 2.89                     | 0.40              |
| 36:5:1507:G:N3     | 36:5:1507:G:H2'    | 2.36                     | 0.40              |
| 36:5:1591:G:OP1    | 70:o4:37:LYS:NZ    | 2.54                     | 0.40              |
| 36:5:1601:U:P      | 55:m9:42:ARG:HH22  | 2.45                     | 0.40              |
| 36:5:1719:G:N7     | 55:m9:121:HIS:HE1  | 2.19                     | 0.40              |
| 36:5:3206:C:O2     | 56:n0:155:ARG:NH1  | 2.54                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:5:3232:G:H2'    | 36:5:3233:C:O4'    | 2.22                     | 0.40              |
| 37:7:76:A:O2'      | 56:n0:50:LYS:NZ    | 2.52                     | 0.40              |
| 39:l2:2:GLY:HA2    | 39:l2:207:VAL:HG12 | 2.04                     | 0.40              |
| 39:l2:140:ASN:OD1  | 39:l2:142:ASP:HB3  | 2.21                     | 0.40              |
| 39:l2:222:ALA:HB1  | 39:l2:224:THR:HG22 | 2.03                     | 0.40              |
| 40:l3:21:ARG:HD3   | 40:l3:269:GLN:OE1  | 2.21                     | 0.40              |
| 40:l3:59:ASP:OD1   | 40:l3:71:GLU:HG2   | 2.21                     | 0.40              |
| 40:l3:169:THR:CG2  | 40:l3:171:LEU:HG   | 2.51                     | 0.40              |
| 42:l5:119:TYR:OH   | 42:l5:141:PRO:HD3  | 2.21                     | 0.40              |
| 45:l8:180:VAL:HG11 | 45:l8:186:LEU:HD21 | 2.01                     | 0.40              |
| 48:m1:94:ARG:HB2   | 48:m1:95:ASN:H     | 1.66                     | 0.40              |
| 57:n1:36:VAL:HA    | 57:n1:64:VAL:HG12  | 2.02                     | 0.40              |
| 70:o4:19:LYS:HB3   | 70:o4:19:LYS:HE2   | 1.89                     | 0.40              |
| 70:o4:20:ILE:HD11  | 70:o4:34:HIS:NE2   | 2.37                     | 0.40              |
| 78:q2:83:LEU:HD23  | 78:q2:83:LEU:HA    | 1.91                     | 0.40              |
| 1:2:325:G:H4'      | 13:C1:83:THR:HG21  | 2.03                     | 0.40              |
| 1:2:448:C:OP1      | 6:S4:29:PRO:HD3    | 2.20                     | 0.40              |
| 1:2:512:A:H5''     | 11:S9:163:PRO:HG3  | 2.02                     | 0.40              |
| 1:2:553:G:C6       | 1:2:554:C:N3       | 2.88                     | 0.40              |
| 1:2:821:U:C5       | 1:2:853:G:N2       | 2.89                     | 0.40              |
| 1:2:953:G:H2'      | 1:2:954:G:C8       | 2.56                     | 0.40              |
| 1:2:1039:A:O2'     | 1:2:1040:G:P       | 2.78                     | 0.40              |
| 1:2:1196:A:H3'     | 1:2:1196:A:OP2     | 2.22                     | 0.40              |
| 1:2:1260:U:C2      | 1:2:1261:G:C8      | 3.10                     | 0.40              |
| 1:2:1544:U:OP1     | 20:C8:136:GLN:NE2  | 2.55                     | 0.40              |
| 3:S1:32:ILE:HD11   | 3:S1:46:THR:HG23   | 2.03                     | 0.40              |
| 4:S2:242:ILE:HG22  | 4:S2:243:TYR:CD2   | 2.55                     | 0.40              |
| 5:S3:172:THR:HA    | 5:S3:184:ILE:O     | 2.20                     | 0.40              |
| 7:S5:56:ALA:O      | 7:S5:57:SER:OG     | 2.29                     | 0.40              |
| 10:S8:146:ARG:O    | 10:S8:147:ALA:HB3  | 2.21                     | 0.40              |
| 17:C5:80:MET:HE2   | 17:C5:80:MET:HB3   | 1.89                     | 0.40              |
| 19:C7:25:THR:C     | 19:C7:27:ASP:H     | 2.30                     | 0.40              |
| 21:C9:28:LEU:HD23  | 21:C9:55:TYR:CE1   | 2.55                     | 0.40              |
| 25:D3:48:HIS:CD2   | 25:D3:105:ALA:HB2  | 2.56                     | 0.40              |
| 28:D6:35:ALA:O     | 28:D6:36:ILE:HG22  | 2.21                     | 0.40              |
| 34:SR:108:SER:OG   | 34:SR:109:ASP:N    | 2.46                     | 0.40              |
| 34:SR:112:SER:CB   | 34:SR:153:GLN:HA   | 2.51                     | 0.40              |
| 35:SM:116:GLU:O    | 35:SM:117:LEU:C    | 2.64                     | 0.40              |
| 36:1:89:A:OP2      | 54:M8:171:LYS:NZ   | 2.55                     | 0.40              |
| 36:1:315:C:OP2     | 72:O6:28:TYR:OH    | 2.30                     | 0.40              |
| 36:1:1282:G:C6     | 36:1:1283:C:C4     | 3.09                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:1:1301:A:H4'   | 36:1:1302:A:O5'   | 2.21                     | 0.40              |
| 36:1:1818:U:H2'   | 36:1:1819:U:O4'   | 2.21                     | 0.40              |
| 36:1:1913:A:N3    | 36:1:2120:A:H2'   | 2.36                     | 0.40              |
| 36:1:2162:U:OP1   | 39:L2:234:LYS:NZ  | 2.50                     | 0.40              |
| 36:1:2314:U:H6    | 36:1:2314:U:H2'   | 1.46                     | 0.40              |
| 36:1:2408:U:C2'   | 36:1:2409:G:H5'   | 2.50                     | 0.40              |
| 36:1:2608:G:O2'   | 36:1:2609:A:H5'   | 2.21                     | 0.40              |
| 36:1:2862:U:H2'   | 36:1:2863:G:O4'   | 2.20                     | 0.40              |
| 36:1:2941:A:N7    | 40:L3:255:TRP:CE2 | 2.89                     | 0.40              |
| 36:1:3094:A:H2'   | 36:1:3095:U:C6    | 2.56                     | 0.40              |
| 37:3:22:A:C6      | 37:3:23:A:C6      | 3.09                     | 0.40              |
| 37:3:27:A:OP2     | 42:L5:57:ASN:HB2  | 2.21                     | 0.40              |
| 40:L3:358:TRP:CZ2 | 40:L3:360:ASP:HA  | 2.56                     | 0.40              |
| 41:L4:26:PHE:HA   | 41:L4:127:ALA:HA  | 2.02                     | 0.40              |
| 42:L5:208:MET:HG2 | 42:L5:223:PHE:CZ  | 2.56                     | 0.40              |
| 45:L8:43:LYS:HD3  | 45:L8:43:LYS:HA   | 1.82                     | 0.40              |
| 47:M0:16:PRO:C    | 47:M0:18:PRO:HD3  | 2.46                     | 0.40              |
| 51:M5:149:ASN:OD1 | 86:M5:304:OHX:N2  | 2.54                     | 0.40              |
| 57:N1:100:LYS:C   | 57:N1:102:ARG:N   | 2.80                     | 0.40              |
| 59:N3:13:ILE:O    | 59:N3:14:SER:C    | 2.65                     | 0.40              |
| 67:O1:12:TYR:O    | 67:O1:72:ARG:HD2  | 2.20                     | 0.40              |
| 70:O4:58:ARG:CG   | 70:O4:58:ARG:NH1  | 2.84                     | 0.40              |
| 79:Q3:50:GLY:O    | 79:Q3:51:ALA:CB   | 2.69                     | 0.40              |
| 1:6:722:G:O2'     | 1:6:723:G:H5''    | 2.21                     | 0.40              |
| 1:6:1098:U:C6     | 1:6:1098:U:H5''   | 2.57                     | 0.40              |
| 1:6:1157:A:OP2    | 86:6:2142:OHX:N1  | 2.53                     | 0.40              |
| 1:6:1671:A:H2'    | 1:6:1672:G:O4'    | 2.22                     | 0.40              |
| 5:s3:113:LEU:HD13 | 5:s3:113:LEU:HA   | 1.90                     | 0.40              |
| 6:s4:21:ASP:CG    | 6:s4:24:SER:HG    | 2.29                     | 0.40              |
| 7:s5:73:THR:C     | 7:s5:75:GLY:H     | 2.28                     | 0.40              |
| 9:s7:21:ALA:O     | 9:s7:24:PHE:HB2   | 2.21                     | 0.40              |
| 12:c0:16:PHE:CD1  | 12:c0:76:LEU:HD12 | 2.56                     | 0.40              |
| 14:c2:125:ASN:HB2 | 35:sM:169:ALA:HB3 | 2.02                     | 0.40              |
| 23:d1:3:ASN:OD1   | 23:d1:3:ASN:C     | 2.64                     | 0.40              |
| 27:d5:44:GLN:HA   | 27:d5:47:TYR:HB3  | 2.03                     | 0.40              |
| 31:d9:37:ASN:C    | 31:d9:38:ILE:HG12 | 2.46                     | 0.40              |
| 34:sR:114:ASP:OD1 | 34:sR:115:ILE:N   | 2.53                     | 0.40              |
| 36:5:238:A:H2'    | 36:5:239:G:O4'    | 2.21                     | 0.40              |
| 36:5:315:C:H5     | 72:o6:28:TYR:HE1  | 1.68                     | 0.40              |
| 36:5:437:G:H1     | 36:5:622:A:N6     | 2.19                     | 0.40              |
| 36:5:619:A:OP2    | 36:5:619:A:H8     | 2.04                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:5:1096:U:H4'   | 36:5:1097:G:O5'    | 2.21                     | 0.40              |
| 36:5:2144:A:H1'   | 36:5:2281:A:N6     | 2.37                     | 0.40              |
| 36:5:2822:U:H2'   | 36:5:2823:G:O4'    | 2.21                     | 0.40              |
| 36:5:3163:A:C5    | 36:5:3164:C:N4     | 2.89                     | 0.40              |
| 86:5:4065:OHX:N2  | 86:5:4074:OHX:N5   | 2.69                     | 0.40              |
| 39:12:44:ILE:HD13 | 39:12:46:LYS:HD2   | 2.03                     | 0.40              |
| 39:12:109:GLU:HA  | 39:12:136:ILE:HG22 | 2.04                     | 0.40              |
| 41:14:319:LYS:O   | 41:14:320:ASN:CB   | 2.66                     | 0.40              |
| 44:17:25:GLN:O    | 44:17:28:ALA:HB3   | 2.21                     | 0.40              |
| 47:m0:74:LYS:HD3  | 47:m0:74:LYS:HA    | 1.85                     | 0.40              |
| 49:m3:46:ILE:HD12 | 49:m3:46:ILE:HG23  | 1.67                     | 0.40              |
| 50:m4:46:ILE:HD13 | 50:m4:58:ILE:HG21  | 2.03                     | 0.40              |
| 64:n8:60:TYR:C    | 64:n8:60:TYR:CD1   | 2.99                     | 0.40              |
| 69:o3:91:ALA:C    | 69:o3:93:THR:H     | 2.28                     | 0.40              |
| 1:2:220:A:H5''    | 1:2:832:U:H1'      | 2.04                     | 0.40              |
| 1:2:540:G:OP2     | 1:2:540:G:H2'      | 2.21                     | 0.40              |
| 1:2:848:C:H2'     | 1:2:849:C:H6       | 1.87                     | 0.40              |
| 1:2:1231:U:O5'    | 1:2:1259:U:H1'     | 2.22                     | 0.40              |
| 1:2:1261:G:H2'    | 1:2:1262:U:C6      | 2.56                     | 0.40              |
| 1:2:1530:C:OP2    | 27:D5:95:HIS:CD2   | 2.74                     | 0.40              |
| 3:S1:62:LYS:C     | 3:S1:64:ARG:H      | 2.26                     | 0.40              |
| 3:S1:128:LYS:HE3  | 3:S1:132:ASP:OD1   | 2.22                     | 0.40              |
| 5:S3:11:LEU:HD12  | 22:D0:86:ILE:HG12  | 2.02                     | 0.40              |
| 7:S5:45:LYS:HA    | 7:S5:45:LYS:HD3    | 1.37                     | 0.40              |
| 10:S8:138:ASN:O   | 10:S8:142:LYS:HG3  | 2.21                     | 0.40              |
| 11:S9:6:ARG:HA    | 11:S9:6:ARG:HD3    | 1.87                     | 0.40              |
| 15:C3:62:GLN:HB2  | 15:C3:65:VAL:HG23  | 2.02                     | 0.40              |
| 17:C5:22:LEU:HD13 | 17:C5:26:LEU:HD11  | 2.03                     | 0.40              |
| 18:C6:109:PHE:O   | 18:C6:113:ASP:N    | 2.55                     | 0.40              |
| 20:C8:14:ILE:HA   | 20:C8:22:VAL:O     | 2.21                     | 0.40              |
| 27:D5:59:TYR:CE2  | 27:D5:100:ILE:HG12 | 2.56                     | 0.40              |
| 28:D6:84:VAL:HG22 | 28:D6:85:ARG:C     | 2.46                     | 0.40              |
| 36:1:200:C:P      | 62:N6:60:ARG:NH1   | 2.95                     | 0.40              |
| 36:1:1573:G:N3    | 36:1:1573:G:H2'    | 2.36                     | 0.40              |
| 36:1:1653:G:H2'   | 36:1:1654:A:O4'    | 2.21                     | 0.40              |
| 36:1:3393:U:O2'   | 36:1:3394:U:H5'    | 2.21                     | 0.40              |
| 38:4:15:G:C6      | 38:4:16:G:N1       | 2.89                     | 0.40              |
| 39:L2:133:TYR:CD2 | 39:L2:168:VAL:HG12 | 2.56                     | 0.40              |
| 43:L6:56:LYS:HD2  | 43:L6:98:VAL:HG13  | 2.02                     | 0.40              |
| 48:M1:16:LYS:HG2  | 48:M1:130:VAL:CG1  | 2.51                     | 0.40              |
| 51:M5:165:THR:O   | 51:M5:169:LYS:HG3  | 2.22                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:M7:36:ILE:HG21  | 53:M7:36:ILE:HD13  | 1.58                     | 0.40              |
| 55:M9:92:GLN:O     | 55:M9:92:GLN:HG2   | 2.22                     | 0.40              |
| 64:N8:79:TRP:CH2   | 64:N8:121:VAL:HG11 | 2.56                     | 0.40              |
| 67:O1:100:SER:OG   | 67:O1:102:LYS:HB3  | 2.22                     | 0.40              |
| 78:Q2:69:VAL:HG22  | 78:Q2:84:THR:HB    | 2.03                     | 0.40              |
| 1:6:484:C:N4       | 1:6:503:G:H22      | 2.18                     | 0.40              |
| 3:s1:93:GLY:C      | 3:s1:95:ASN:H      | 2.29                     | 0.40              |
| 5:s3:196:ARG:HB3   | 5:s3:197:THR:H     | 1.73                     | 0.40              |
| 7:s5:172:ILE:O     | 7:s5:176:THR:HG23  | 2.20                     | 0.40              |
| 8:s6:116:LYS:NZ    | 8:s6:120:GLU:OE1   | 2.46                     | 0.40              |
| 8:s6:173:PRO:HB2   | 8:s6:174:LYS:H     | 1.46                     | 0.40              |
| 14:c2:67:THR:O     | 14:c2:68:GLU:HB2   | 2.21                     | 0.40              |
| 15:c3:36:GLN:NE2   | 15:c3:39:LYS:HD2   | 2.37                     | 0.40              |
| 15:c3:119:GLU:O    | 15:c3:123:HIS:ND1  | 2.49                     | 0.40              |
| 25:d3:31:LYS:HD3   | 25:d3:31:LYS:HA    | 1.84                     | 0.40              |
| 27:d5:47:TYR:CE1   | 27:d5:51:LEU:HD11  | 2.56                     | 0.40              |
| 29:d7:75:GLU:HB3   | 29:d7:76:GLY:H     | 1.57                     | 0.40              |
| 36:5:349:A:O4'     | 38:8:24:G:H1'      | 2.20                     | 0.40              |
| 36:5:627:U:H4'     | 36:5:1399:A:O2'    | 2.22                     | 0.40              |
| 36:5:683:U:H5''    | 51:m5:200:TRP:CZ3  | 2.56                     | 0.40              |
| 36:5:726:G:C5'     | 36:5:726:G:C8      | 3.04                     | 0.40              |
| 36:5:734:C:H2'     | 36:5:735:A:O4'     | 2.21                     | 0.40              |
| 36:5:785:G:N7      | 64:n8:77:LYS:NZ    | 2.70                     | 0.40              |
| 36:5:792:G:H2'     | 36:5:793:C:C6      | 2.56                     | 0.40              |
| 36:5:1340:G:H2'    | 36:5:1341:U:C6     | 2.56                     | 0.40              |
| 36:5:1746:U:O2'    | 74:o8:4:GLU:OE1    | 2.39                     | 0.40              |
| 36:5:2572:C:O2'    | 36:5:2573:G:OP2    | 2.38                     | 0.40              |
| 86:5:4187:OHX:N3   | 86:5:4189:OHX:N6   | 2.69                     | 0.40              |
| 88:5:4251:3H3:C9   | 88:5:4251:3H3:C3   | 2.99                     | 0.40              |
| 40:l3:252:ILE:HD12 | 40:l3:252:ILE:HA   | 1.70                     | 0.40              |
| 45:l8:67:ILE:HA    | 45:l8:67:ILE:HD13  | 1.65                     | 0.40              |
| 81:m2:54:UNK:HA    | 81:m2:55:UNK:HA    | 1.86                     | 0.40              |
| 64:n8:46:ASP:O     | 64:n8:47:LYS:O     | 2.39                     | 0.40              |
| 71:o5:114:ARG:HA   | 71:o5:114:ARG:HD2  | 1.87                     | 0.40              |
| 72:o6:40:VAL:O     | 72:o6:44:VAL:HG23  | 2.21                     | 0.40              |
| 82:p0:198:PRO:HG2  | 82:p0:201:ILE:H    | 1.85                     | 0.40              |
| 1:2:113:U:H4'      | 1:2:115:G:OP1      | 2.22                     | 0.40              |
| 1:2:548:G:H2'      | 1:2:549:G:O4'      | 2.21                     | 0.40              |
| 1:2:778:G:N2       | 1:2:780:A:C6       | 2.90                     | 0.40              |
| 1:2:1199:G:O6      | 31:D9:31:ILE:HD11  | 2.21                     | 0.40              |
| 1:2:1291:G:H1      | 1:2:1324:G:H22     | 1.69                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2:1409:G:N2      | 1:2:1411:A:H3'     | 2.37                     | 0.40              |
| 2:S0:35:PRO:HG3    | 23:D1:87:ARG:NH2   | 2.37                     | 0.40              |
| 4:S2:61:LEU:HA     | 4:S2:62:PRO:HD2    | 1.97                     | 0.40              |
| 4:S2:121:VAL:O     | 4:S2:125:ILE:HG13  | 2.21                     | 0.40              |
| 4:S2:170:ILE:HA    | 4:S2:171:PRO:HD3   | 1.86                     | 0.40              |
| 4:S2:235:LEU:HD11  | 23:D1:54:ALA:HB2   | 2.02                     | 0.40              |
| 10:S8:136:SER:HB3  | 10:S8:139:ALA:CB   | 2.52                     | 0.40              |
| 17:C5:98:ASN:C     | 17:C5:98:ASN:OD1   | 2.64                     | 0.40              |
| 19:C7:82:ASP:O     | 19:C7:83:GLN:HB2   | 2.21                     | 0.40              |
| 23:D1:5:LYS:O      | 23:D1:7:GLN:N      | 2.54                     | 0.40              |
| 26:D4:40:LEU:O     | 26:D4:44:LEU:HB2   | 2.22                     | 0.40              |
| 36:1:671:U:O2'     | 54:M8:20:LYS:HD3   | 2.21                     | 0.40              |
| 36:1:1106:G:H2'    | 36:1:1107:C:O4'    | 2.22                     | 0.40              |
| 36:1:1230:G:OP2    | 86:1:4089:OHX:N2   | 2.55                     | 0.40              |
| 36:1:2257:C:H2'    | 36:1:2258:U:O4'    | 2.21                     | 0.40              |
| 36:1:2567:C:C2'    | 36:1:2568:C:H5'    | 2.52                     | 0.40              |
| 36:1:2656:A:C8     | 36:1:2658:G:C8     | 3.10                     | 0.40              |
| 36:1:2777:G:H5''   | 36:1:2778:G:OP1    | 2.21                     | 0.40              |
| 36:1:3271:G:OP1    | 53:M7:171:ARG:HG2  | 2.22                     | 0.40              |
| 36:1:3366:G:H2'    | 36:1:3367:C:C6     | 2.56                     | 0.40              |
| 36:1:3375:A:H5''   | 36:1:3378:C:H5     | 1.85                     | 0.40              |
| 39:L2:77:ILE:HD13  | 39:L2:128:ARG:HB3  | 2.03                     | 0.40              |
| 40:L3:255:TRP:HD1  | 40:L3:255:TRP:O    | 2.04                     | 0.40              |
| 44:L7:158:LYS:CE   | 44:L7:159:GLN:H    | 2.34                     | 0.40              |
| 49:M3:149:GLN:HA   | 49:M3:150:PRO:HD3  | 1.90                     | 0.40              |
| 52:M6:181:ALA:O    | 52:M6:183:ALA:N    | 2.54                     | 0.40              |
| 64:N8:44:ASN:O     | 64:N8:47:LYS:O     | 2.40                     | 0.40              |
| 64:N8:121:VAL:HA   | 64:N8:122:PRO:HD3  | 1.94                     | 0.40              |
| 72:O6:54:GLU:HG2   | 72:O6:90:MET:HE3   | 2.02                     | 0.40              |
| 73:O7:87:SER:C     | 86:O7:103:OHX:N1   | 2.80                     | 0.40              |
| 1:6:198:A:C2'      | 1:6:199:G:H5'      | 2.51                     | 0.40              |
| 1:6:607:G:H5'      | 1:6:613:G:N2       | 2.37                     | 0.40              |
| 1:6:1102:G:H2'     | 1:6:1103:U:O4'     | 2.21                     | 0.40              |
| 1:6:1146:G:C6      | 1:6:1147:A:C6      | 3.09                     | 0.40              |
| 1:6:1559:A:H5''    | 20:c8:135:GLY:HA3  | 2.04                     | 0.40              |
| 1:6:1614:A:C6      | 1:6:1615:C:N4      | 2.89                     | 0.40              |
| 1:6:1619:C:O2      | 30:d8:22:ARG:HD2   | 2.20                     | 0.40              |
| 4:s2:98:PHE:CD2    | 4:s2:121:VAL:HG23  | 2.56                     | 0.40              |
| 5:s3:157:LEU:HD23  | 5:s3:189:MET:HB2   | 2.02                     | 0.40              |
| 6:s4:85:GLY:N      | 6:s4:88:ASP:OD2    | 2.38                     | 0.40              |
| 11:s9:113:VAL:HG21 | 11:s9:134:ILE:HG21 | 2.04                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:c2:81:ASP:HA    | 14:c2:82:PRO:HD2  | 1.95                     | 0.40              |
| 15:c3:54:LEU:HB3   | 15:c3:60:VAL:HG11 | 2.03                     | 0.40              |
| 20:c8:8:GLN:C      | 20:c8:10:SER:H    | 2.30                     | 0.40              |
| 20:c8:31:ALA:CB    | 20:c8:58:ALA:HB2  | 2.51                     | 0.40              |
| 27:d5:38:HIS:HB3   | 27:d5:39:ALA:H    | 1.59                     | 0.40              |
| 36:5:260:C:H2'     | 36:5:261:U:C6     | 2.57                     | 0.40              |
| 36:5:715:A:H4'     | 36:5:716:A:OP1    | 2.21                     | 0.40              |
| 36:5:1313:G:H2'    | 36:5:1314:C:C6    | 2.57                     | 0.40              |
| 36:5:2211:U:H5     | 36:5:2234:G:C6    | 2.39                     | 0.40              |
| 36:5:2623:G:H2'    | 36:5:2624:G:O4'   | 2.21                     | 0.40              |
| 36:5:2772:C:H1'    | 36:5:2773:C:OP2   | 2.22                     | 0.40              |
| 36:5:3182:G:H2'    | 36:5:3183:A:O4'   | 2.20                     | 0.40              |
| 39:l2:180:LEU:HD23 | 39:l2:180:LEU:HA  | 1.80                     | 0.40              |
| 45:l8:156:ASP:OD1  | 45:l8:183:LYS:HG2 | 2.20                     | 0.40              |
| 46:l9:94:TYR:CD2   | 46:l9:98:PRO:HA   | 2.56                     | 0.40              |
| 48:m1:108:GLU:HA   | 48:m1:122:ILE:CG2 | 2.51                     | 0.40              |
| 51:m5:67:ARG:O     | 51:m5:68:ARG:HB3  | 2.20                     | 0.40              |
| 53:m7:65:SER:O     | 53:m7:66:SER:HB2  | 2.21                     | 0.40              |
| 54:m8:147:ARG:H    | 54:m8:147:ARG:HG2 | 1.55                     | 0.40              |
| 59:n3:128:ARG:CZ   | 59:n3:128:ARG:HB3 | 2.51                     | 0.40              |
| 64:n8:60:TYR:C     | 64:n8:60:TYR:HD1  | 2.30                     | 0.40              |
| 70:o4:94:LEU:HA    | 70:o4:94:LEU:HD23 | 1.74                     | 0.40              |
| 1:2:1:U:O4         | 11:S9:54:ARG:HD3  | 2.21                     | 0.40              |
| 1:2:93:A:HO2'      | 6:S4:4:GLY:HA3    | 1.85                     | 0.40              |
| 1:2:119:A:H1'      | 1:2:397:A:C5      | 2.56                     | 0.40              |
| 1:2:180:A:H2'      | 1:2:181:A:O4'     | 2.21                     | 0.40              |
| 1:2:976:G:C6       | 1:2:1023:A:C4     | 3.10                     | 0.40              |
| 1:2:1369:U:OP2     | 21:C9:69:LYS:HE3  | 2.22                     | 0.40              |
| 1:2:1553:G:HO2'    | 31:D9:14:TYR:HH   | 1.62                     | 0.40              |
| 2:S0:202:TYR:O     | 2:S0:203:PHE:CG   | 2.74                     | 0.40              |
| 6:S4:48:LEU:HD12   | 6:S4:48:LEU:HA    | 1.80                     | 0.40              |
| 7:S5:39:GLU:HB3    | 7:S5:40:ILE:H     | 1.68                     | 0.40              |
| 8:S6:31:ARG:HE     | 8:S6:68:LEU:CD1   | 2.34                     | 0.40              |
| 12:C0:29:GLN:O     | 12:C0:30:ALA:HB3  | 2.21                     | 0.40              |
| 14:C2:131:ASP:OD1  | 14:C2:132:GLU:N   | 2.49                     | 0.40              |
| 16:C4:42:VAL:HA    | 16:C4:46:MET:SD   | 2.62                     | 0.40              |
| 20:C8:8:GLN:HB2    | 20:C8:9:GLY:H     | 1.51                     | 0.40              |
| 22:D0:29:THR:OG1   | 22:D0:30:LYS:HE2  | 2.21                     | 0.40              |
| 22:D0:63:LEU:O     | 22:D0:83:GLU:HA   | 2.21                     | 0.40              |
| 25:D3:7:ARG:HH11   | 25:D3:7:ARG:CG    | 2.34                     | 0.40              |
| 27:D5:59:TYR:CD2   | 27:D5:59:TYR:C    | 2.99                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:D5:83:LEU:HD23  | 27:D5:83:LEU:HA    | 1.81                     | 0.40              |
| 28:D6:37:LYS:HD3   | 28:D6:70:LYS:NZ    | 2.36                     | 0.40              |
| 29:D7:36:LYS:HB3   | 29:D7:43:ILE:HG23  | 2.03                     | 0.40              |
| 36:1:38:U:H2'      | 36:1:39:A:O4'      | 2.21                     | 0.40              |
| 36:1:128:G:H2'     | 36:1:129:U:O4'     | 2.22                     | 0.40              |
| 36:1:1083:G:C6     | 36:1:1084:A:C6     | 3.09                     | 0.40              |
| 36:1:1549:U:H2'    | 36:1:1550:C:C6     | 2.56                     | 0.40              |
| 36:1:1569:U:H5''   | 36:1:1570:U:H5''   | 2.04                     | 0.40              |
| 36:1:1765:U:H2'    | 36:1:1766:G:C8     | 2.57                     | 0.40              |
| 36:1:2655:U:H2'    | 78:Q2:3:ASN:O      | 2.21                     | 0.40              |
| 36:1:3006:A:OP2    | 52:M6:148:LYS:NZ   | 2.41                     | 0.40              |
| 86:1:4065:OHX:N4   | 86:1:4177:OHX:N1   | 2.70                     | 0.40              |
| 41:L4:16:THR:C     | 41:L4:18:ASN:H     | 2.29                     | 0.40              |
| 42:L5:111:GLN:O    | 42:L5:113:LEU:N    | 2.55                     | 0.40              |
| 45:L8:149:LYS:O    | 45:L8:176:PRO:HG2  | 2.22                     | 0.40              |
| 46:L9:84:LYS:NZ    | 46:L9:191:LEU:HD13 | 2.36                     | 0.40              |
| 48:M1:9:MET:C      | 48:M1:11:ASP:H     | 2.29                     | 0.40              |
| 48:M1:60:ARG:HB2   | 48:M1:60:ARG:NH1   | 2.36                     | 0.40              |
| 54:M8:70:ALA:HB1   | 54:M8:138:LEU:HD11 | 2.03                     | 0.40              |
| 54:M8:176:ARG:NH1  | 64:N8:46:ASP:OD2   | 2.55                     | 0.40              |
| 56:N0:81:TYR:CE1   | 56:N0:88:HIS:HB2   | 2.56                     | 0.40              |
| 57:N1:88:ARG:NH2   | 65:N9:33:LYS:O     | 2.34                     | 0.40              |
| 58:N2:21:SER:HA    | 58:N2:24:GLU:OE2   | 2.22                     | 0.40              |
| 64:N8:131:SER:O    | 64:N8:132:LYS:C    | 2.64                     | 0.40              |
| 71:O5:21:LEU:HD21  | 71:O5:51:ILE:HG23  | 2.03                     | 0.40              |
| 1:6:449:C:OP1      | 6:s4:29:PRO:O      | 2.39                     | 0.40              |
| 1:6:454:U:C4       | 6:s4:66:MET:HB3    | 2.56                     | 0.40              |
| 1:6:481:A:C2       | 1:6:508:U:C2       | 3.09                     | 0.40              |
| 1:6:548:G:H2'      | 1:6:549:G:O4'      | 2.22                     | 0.40              |
| 1:6:634:G:H2'      | 1:6:635:A:OP2      | 2.22                     | 0.40              |
| 1:6:765:G:N7       | 11:s9:149:ARG:CZ   | 2.84                     | 0.40              |
| 1:6:922:G:H2'      | 1:6:923:A:C8       | 2.57                     | 0.40              |
| 1:6:1208:A:H5''    | 1:6:1209:C:OP2     | 2.22                     | 0.40              |
| 1:6:1344:A:O2'     | 1:6:1345:A:OP1     | 2.36                     | 0.40              |
| 9:s7:157:LYS:HB2   | 9:s7:157:LYS:HE3   | 1.82                     | 0.40              |
| 10:s8:61:GLU:OE2   | 10:s8:77:ARG:NH1   | 2.54                     | 0.40              |
| 11:s9:150:LEU:HD12 | 11:s9:150:LEU:HA   | 1.68                     | 0.40              |
| 14:c2:57:ALA:O     | 14:c2:85:LYS:HE3   | 2.22                     | 0.40              |
| 17:c5:126:VAL:HG13 | 17:c5:127:ARG:N    | 2.36                     | 0.40              |
| 22:d0:72:ASN:CG    | 22:d0:73:GLY:N     | 2.79                     | 0.40              |
| 22:d0:99:ILE:H     | 22:d0:99:ILE:HG12  | 1.48                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:d2:21:GLY:O    | 29:d7:3:LEU:HD22  | 2.21                     | 0.40              |
| 27:d5:49:ARG:O    | 27:d5:53:GLU:HB2  | 2.22                     | 0.40              |
| 29:d7:30:SER:HB2  | 29:d7:48:SER:OG   | 2.21                     | 0.40              |
| 31:d9:19:ARG:HD2  | 31:d9:32:ARG:HD2  | 2.04                     | 0.40              |
| 35:sM:71:ASN:C    | 35:sM:73:SER:H    | 2.29                     | 0.40              |
| 36:5:119:U:H4'    | 36:5:120:G:H3'    | 2.04                     | 0.40              |
| 36:5:1221:A:H4'   | 36:5:1222:G:OP2   | 2.22                     | 0.40              |
| 36:5:2767:U:H2'   | 36:5:2768:U:C6    | 2.57                     | 0.40              |
| 36:5:2770:G:C2'   | 36:5:2771:U:H5'   | 2.51                     | 0.40              |
| 36:5:2931:C:OP1   | 59:n3:59:MET:HE2  | 2.21                     | 0.40              |
| 45:l8:167:PRO:HB3 | 45:l8:177:TYR:CE1 | 2.56                     | 0.40              |
| 51:m5:163:GLY:CA  | 51:m5:168:GLY:HA3 | 2.50                     | 0.40              |
| 54:m8:58:ASN:HB3  | 54:m8:144:ARG:NH2 | 2.36                     | 0.40              |
| 56:n0:38:LYS:HB2  | 56:n0:38:LYS:HE3  | 1.92                     | 0.40              |
| 63:n7:81:LEU:HA   | 63:n7:81:LEU:HD22 | 1.89                     | 0.40              |
| 64:n8:119:PRO:O   | 64:n8:121:VAL:N   | 2.55                     | 0.40              |
| 76:q0:92:ASP:C    | 76:q0:93:LYS:HG2  | 2.47                     | 0.40              |
| 82:p0:15:LEU:O    | 82:p0:19:LEU:HG   | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2   | S0    | 204/251 (81%) | 154 (76%) | 27 (13%) | 23 (11%) | 0           | 1 |
| 2   | s0    | 204/251 (81%) | 161 (79%) | 27 (13%) | 16 (8%)  | 1           | 2 |
| 3   | S1    | 212/254 (84%) | 152 (72%) | 31 (15%) | 29 (14%) | 0           | 0 |
| 3   | s1    | 214/254 (84%) | 179 (84%) | 23 (11%) | 12 (6%)  | 1           | 4 |
| 4   | S2    | 215/253 (85%) | 181 (84%) | 25 (12%) | 9 (4%)   | 2           | 7 |
| 4   | s2    | 215/253 (85%) | 187 (87%) | 16 (7%)  | 12 (6%)  | 1           | 4 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5   | S3    | 221/239 (92%) | 198 (90%) | 14 (6%)  | 9 (4%)   | 2           | 8  |
| 5   | s3    | 221/239 (92%) | 193 (87%) | 15 (7%)  | 13 (6%)  | 1           | 3  |
| 6   | S4    | 258/260 (99%) | 219 (85%) | 27 (10%) | 12 (5%)  | 2           | 6  |
| 6   | s4    | 258/260 (99%) | 223 (86%) | 23 (9%)  | 12 (5%)  | 2           | 6  |
| 7   | S5    | 204/224 (91%) | 162 (79%) | 21 (10%) | 21 (10%) | 0           | 1  |
| 7   | s5    | 204/224 (91%) | 164 (80%) | 23 (11%) | 17 (8%)  | 0           | 1  |
| 8   | S6    | 224/236 (95%) | 195 (87%) | 21 (9%)  | 8 (4%)   | 2           | 10 |
| 8   | s6    | 216/236 (92%) | 194 (90%) | 14 (6%)  | 8 (4%)   | 2           | 9  |
| 9   | S7    | 182/189 (96%) | 143 (79%) | 21 (12%) | 18 (10%) | 0           | 1  |
| 9   | s7    | 184/189 (97%) | 148 (80%) | 22 (12%) | 14 (8%)  | 1           | 2  |
| 10  | S8    | 184/200 (92%) | 159 (86%) | 12 (6%)  | 13 (7%)  | 1           | 2  |
| 10  | s8    | 184/200 (92%) | 164 (89%) | 11 (6%)  | 9 (5%)   | 1           | 6  |
| 11  | S9    | 183/196 (93%) | 159 (87%) | 15 (8%)  | 9 (5%)   | 1           | 6  |
| 11  | s9    | 183/196 (93%) | 148 (81%) | 23 (13%) | 12 (7%)  | 1           | 3  |
| 12  | C0    | 94/105 (90%)  | 74 (79%)  | 14 (15%) | 6 (6%)   | 1           | 3  |
| 12  | c0    | 92/105 (88%)  | 63 (68%)  | 16 (17%) | 13 (14%) | 0           | 0  |
| 13  | C1    | 153/155 (99%) | 125 (82%) | 18 (12%) | 10 (6%)  | 1           | 3  |
| 13  | c1    | 144/155 (93%) | 117 (81%) | 18 (12%) | 9 (6%)   | 1           | 3  |
| 14  | C2    | 122/142 (86%) | 70 (57%)  | 26 (21%) | 26 (21%) | 0           | 0  |
| 14  | c2    | 122/142 (86%) | 71 (58%)  | 29 (24%) | 22 (18%) | 0           | 0  |
| 15  | C3    | 148/150 (99%) | 132 (89%) | 13 (9%)  | 3 (2%)   | 6           | 21 |
| 15  | c3    | 148/150 (99%) | 123 (83%) | 16 (11%) | 9 (6%)   | 1           | 3  |
| 16  | C4    | 125/136 (92%) | 97 (78%)  | 16 (13%) | 12 (10%) | 0           | 1  |
| 16  | c4    | 126/136 (93%) | 101 (80%) | 15 (12%) | 10 (8%)  | 1           | 1  |
| 17  | C5    | 122/141 (86%) | 95 (78%)  | 16 (13%) | 11 (9%)  | 0           | 1  |
| 17  | c5    | 133/141 (94%) | 97 (73%)  | 16 (12%) | 20 (15%) | 0           | 0  |
| 18  | C6    | 139/142 (98%) | 121 (87%) | 13 (9%)  | 5 (4%)   | 2           | 10 |
| 18  | c6    | 140/142 (99%) | 121 (86%) | 11 (8%)  | 8 (6%)   | 1           | 4  |
| 19  | C7    | 116/136 (85%) | 87 (75%)  | 22 (19%) | 7 (6%)   | 1           | 3  |
| 19  | c7    | 113/136 (83%) | 96 (85%)  | 11 (10%) | 6 (5%)   | 1           | 5  |
| 20  | C8    | 143/145 (99%) | 121 (85%) | 11 (8%)  | 11 (8%)  | 1           | 2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 20  | c8    | 143/145 (99%) | 115 (80%) | 21 (15%) | 7 (5%)   | 1           | 6  |
| 21  | C9    | 141/143 (99%) | 122 (86%) | 14 (10%) | 5 (4%)   | 3           | 10 |
| 21  | c9    | 141/143 (99%) | 122 (86%) | 14 (10%) | 5 (4%)   | 3           | 10 |
| 22  | D0    | 105/120 (88%) | 88 (84%)  | 15 (14%) | 2 (2%)   | 6           | 22 |
| 22  | d0    | 108/120 (90%) | 85 (79%)  | 15 (14%) | 8 (7%)   | 1           | 2  |
| 23  | D1    | 85/87 (98%)   | 69 (81%)  | 10 (12%) | 6 (7%)   | 1           | 2  |
| 23  | d1    | 85/87 (98%)   | 75 (88%)  | 5 (6%)   | 5 (6%)   | 1           | 3  |
| 24  | D2    | 127/129 (98%) | 113 (89%) | 13 (10%) | 1 (1%)   | 16          | 44 |
| 24  | d2    | 127/129 (98%) | 116 (91%) | 10 (8%)  | 1 (1%)   | 16          | 44 |
| 25  | D3    | 142/144 (99%) | 117 (82%) | 14 (10%) | 11 (8%)  | 1           | 2  |
| 25  | d3    | 142/144 (99%) | 131 (92%) | 10 (7%)  | 1 (1%)   | 18          | 47 |
| 26  | D4    | 132/134 (98%) | 110 (83%) | 14 (11%) | 8 (6%)   | 1           | 3  |
| 26  | d4    | 132/134 (98%) | 106 (80%) | 15 (11%) | 11 (8%)  | 0           | 1  |
| 27  | D5    | 68/107 (64%)  | 51 (75%)  | 9 (13%)  | 8 (12%)  | 0           | 1  |
| 27  | d5    | 67/107 (63%)  | 48 (72%)  | 13 (19%) | 6 (9%)   | 0           | 1  |
| 28  | D6    | 95/97 (98%)   | 69 (73%)  | 12 (13%) | 14 (15%) | 0           | 0  |
| 28  | d6    | 95/97 (98%)   | 73 (77%)  | 14 (15%) | 8 (8%)   | 0           | 1  |
| 29  | D7    | 79/81 (98%)   | 62 (78%)  | 12 (15%) | 5 (6%)   | 1           | 3  |
| 29  | d7    | 79/81 (98%)   | 60 (76%)  | 10 (13%) | 9 (11%)  | 0           | 1  |
| 30  | D8    | 61/66 (92%)   | 51 (84%)  | 7 (12%)  | 3 (5%)   | 1           | 6  |
| 30  | d8    | 61/66 (92%)   | 46 (75%)  | 10 (16%) | 5 (8%)   | 0           | 1  |
| 31  | D9    | 51/55 (93%)   | 41 (80%)  | 7 (14%)  | 3 (6%)   | 1           | 3  |
| 31  | d9    | 51/55 (93%)   | 42 (82%)  | 5 (10%)  | 4 (8%)   | 1           | 2  |
| 32  | E0    | 58/60 (97%)   | 45 (78%)  | 12 (21%) | 1 (2%)   | 7           | 25 |
| 33  | E1    | 69/76 (91%)   | 36 (52%)  | 14 (20%) | 19 (28%) | 0           | 0  |
| 33  | e1    | 74/76 (97%)   | 38 (51%)  | 16 (22%) | 20 (27%) | 0           | 0  |
| 34  | SR    | 316/318 (99%) | 274 (87%) | 29 (9%)  | 13 (4%)  | 2           | 8  |
| 34  | sR    | 316/318 (99%) | 268 (85%) | 40 (13%) | 8 (2%)   | 4           | 16 |
| 35  | SM    | 155/273 (57%) | 109 (70%) | 26 (17%) | 20 (13%) | 0           | 0  |
| 35  | sM    | 98/273 (36%)  | 61 (62%)  | 24 (24%) | 13 (13%) | 0           | 0  |
| 39  | L2    | 250/253 (99%) | 226 (90%) | 20 (8%)  | 4 (2%)   | 7           | 27 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 39  | l2    | 250/253 (99%)  | 214 (86%) | 27 (11%) | 9 (4%)   | 2           | 10 |
| 40  | L3    | 384/386 (100%) | 340 (88%) | 31 (8%)  | 13 (3%)  | 3           | 11 |
| 40  | l3    | 384/386 (100%) | 350 (91%) | 25 (6%)  | 9 (2%)   | 5           | 18 |
| 41  | L4    | 359/361 (99%)  | 315 (88%) | 23 (6%)  | 21 (6%)  | 1           | 4  |
| 41  | l4    | 359/361 (99%)  | 308 (86%) | 38 (11%) | 13 (4%)  | 2           | 10 |
| 42  | L5    | 294/296 (99%)  | 253 (86%) | 23 (8%)  | 18 (6%)  | 1           | 3  |
| 42  | l5    | 292/296 (99%)  | 262 (90%) | 21 (7%)  | 9 (3%)   | 3           | 12 |
| 43  | L6    | 152/175 (87%)  | 141 (93%) | 8 (5%)   | 3 (2%)   | 6           | 21 |
| 43  | l6    | 153/175 (87%)  | 132 (86%) | 17 (11%) | 4 (3%)   | 4           | 15 |
| 44  | L7    | 220/243 (90%)  | 205 (93%) | 6 (3%)   | 9 (4%)   | 2           | 8  |
| 44  | l7    | 221/243 (91%)  | 203 (92%) | 15 (7%)  | 3 (1%)   | 9           | 30 |
| 45  | L8    | 231/255 (91%)  | 193 (84%) | 30 (13%) | 8 (4%)   | 3           | 10 |
| 45  | l8    | 229/255 (90%)  | 184 (80%) | 25 (11%) | 20 (9%)  | 0           | 1  |
| 46  | L9    | 189/191 (99%)  | 170 (90%) | 14 (7%)  | 5 (3%)   | 4           | 15 |
| 46  | l9    | 189/191 (99%)  | 173 (92%) | 10 (5%)  | 6 (3%)   | 3           | 11 |
| 47  | M0    | 207/220 (94%)  | 185 (89%) | 17 (8%)  | 5 (2%)   | 4           | 17 |
| 47  | m0    | 209/220 (95%)  | 181 (87%) | 20 (10%) | 8 (4%)   | 2           | 9  |
| 48  | M1    | 167/173 (96%)  | 133 (80%) | 20 (12%) | 14 (8%)  | 0           | 1  |
| 48  | m1    | 167/173 (96%)  | 146 (87%) | 11 (7%)  | 10 (6%)  | 1           | 3  |
| 49  | M3    | 191/198 (96%)  | 164 (86%) | 19 (10%) | 8 (4%)   | 2           | 7  |
| 49  | m3    | 192/198 (97%)  | 164 (85%) | 17 (9%)  | 11 (6%)  | 1           | 4  |
| 50  | M4    | 134/137 (98%)  | 118 (88%) | 11 (8%)  | 5 (4%)   | 2           | 9  |
| 50  | m4    | 135/137 (98%)  | 127 (94%) | 6 (4%)   | 2 (2%)   | 8           | 28 |
| 51  | M5    | 201/203 (99%)  | 188 (94%) | 7 (4%)   | 6 (3%)   | 3           | 12 |
| 51  | m5    | 201/203 (99%)  | 180 (90%) | 14 (7%)  | 7 (4%)   | 3           | 10 |
| 52  | M6    | 195/198 (98%)  | 185 (95%) | 6 (3%)   | 4 (2%)   | 5           | 20 |
| 52  | m6    | 195/198 (98%)  | 185 (95%) | 8 (4%)   | 2 (1%)   | 12          | 38 |
| 53  | M7    | 181/183 (99%)  | 159 (88%) | 16 (9%)  | 6 (3%)   | 3           | 11 |
| 53  | m7    | 153/183 (84%)  | 140 (92%) | 10 (6%)  | 3 (2%)   | 6           | 21 |
| 54  | M8    | 183/185 (99%)  | 169 (92%) | 10 (6%)  | 4 (2%)   | 5           | 19 |
| 54  | m8    | 183/185 (99%)  | 165 (90%) | 11 (6%)  | 7 (4%)   | 2           | 9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 55  | M9    | 186/188 (99%) | 173 (93%) | 12 (6%)  | 1 (0%)   | 24          | 55 |
| 55  | m9    | 186/188 (99%) | 175 (94%) | 8 (4%)   | 3 (2%)   | 7           | 27 |
| 56  | N0    | 170/172 (99%) | 157 (92%) | 11 (6%)  | 2 (1%)   | 10          | 34 |
| 56  | n0    | 170/172 (99%) | 158 (93%) | 9 (5%)   | 3 (2%)   | 6           | 23 |
| 57  | N1    | 157/159 (99%) | 138 (88%) | 14 (9%)  | 5 (3%)   | 3           | 11 |
| 57  | n1    | 157/159 (99%) | 143 (91%) | 10 (6%)  | 4 (2%)   | 4           | 16 |
| 58  | N2    | 98/120 (82%)  | 79 (81%)  | 15 (15%) | 4 (4%)   | 2           | 8  |
| 58  | n2    | 96/120 (80%)  | 84 (88%)  | 9 (9%)   | 3 (3%)   | 3           | 12 |
| 59  | N3    | 134/136 (98%) | 126 (94%) | 7 (5%)   | 1 (1%)   | 18          | 47 |
| 59  | n3    | 134/136 (98%) | 125 (93%) | 8 (6%)   | 1 (1%)   | 18          | 47 |
| 60  | N4    | 96/155 (62%)  | 77 (80%)  | 14 (15%) | 5 (5%)   | 1           | 5  |
| 60  | n4    | 133/155 (86%) | 113 (85%) | 12 (9%)  | 8 (6%)   | 1           | 3  |
| 61  | N5    | 119/141 (84%) | 110 (92%) | 8 (7%)   | 1 (1%)   | 16          | 44 |
| 61  | n5    | 118/141 (84%) | 100 (85%) | 13 (11%) | 5 (4%)   | 2           | 7  |
| 62  | N6    | 124/126 (98%) | 114 (92%) | 6 (5%)   | 4 (3%)   | 3           | 11 |
| 62  | n6    | 124/126 (98%) | 113 (91%) | 6 (5%)   | 5 (4%)   | 2           | 8  |
| 63  | N7    | 133/135 (98%) | 111 (84%) | 12 (9%)  | 10 (8%)  | 1           | 2  |
| 63  | n7    | 133/135 (98%) | 111 (84%) | 14 (10%) | 8 (6%)   | 1           | 3  |
| 64  | N8    | 146/148 (99%) | 122 (84%) | 16 (11%) | 8 (6%)   | 1           | 4  |
| 64  | n8    | 146/148 (99%) | 126 (86%) | 16 (11%) | 4 (3%)   | 4           | 15 |
| 65  | N9    | 56/58 (97%)   | 49 (88%)  | 5 (9%)   | 2 (4%)   | 2           | 10 |
| 65  | n9    | 56/58 (97%)   | 43 (77%)  | 9 (16%)  | 4 (7%)   | 1           | 2  |
| 66  | O0    | 95/104 (91%)  | 87 (92%)  | 6 (6%)   | 2 (2%)   | 5           | 20 |
| 66  | o0    | 98/104 (94%)  | 89 (91%)  | 7 (7%)   | 2 (2%)   | 6           | 21 |
| 67  | O1    | 107/112 (96%) | 95 (89%)  | 7 (6%)   | 5 (5%)   | 2           | 6  |
| 67  | o1    | 107/112 (96%) | 98 (92%)  | 5 (5%)   | 4 (4%)   | 2           | 9  |
| 68  | O2    | 125/129 (97%) | 116 (93%) | 8 (6%)   | 1 (1%)   | 16          | 44 |
| 68  | o2    | 125/129 (97%) | 111 (89%) | 11 (9%)  | 3 (2%)   | 4           | 17 |
| 69  | O3    | 104/106 (98%) | 101 (97%) | 2 (2%)   | 1 (1%)   | 12          | 38 |
| 69  | o3    | 104/106 (98%) | 92 (88%)  | 7 (7%)   | 5 (5%)   | 2           | 6  |
| 70  | O4    | 110/119 (92%) | 103 (94%) | 4 (4%)   | 3 (3%)   | 4           | 15 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers  | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|-----------|-------------|-----|
| 70  | o4    | 110/119 (92%)     | 100 (91%)   | 8 (7%)    | 2 (2%)    | 6           | 23  |
| 71  | O5    | 117/119 (98%)     | 108 (92%)   | 5 (4%)    | 4 (3%)    | 3           | 11  |
| 71  | o5    | 117/119 (98%)     | 106 (91%)   | 9 (8%)    | 2 (2%)    | 7           | 25  |
| 72  | O6    | 97/99 (98%)       | 78 (80%)    | 11 (11%)  | 8 (8%)    | 0           | 1   |
| 72  | o6    | 97/99 (98%)       | 81 (84%)    | 9 (9%)    | 7 (7%)    | 1           | 2   |
| 73  | O7    | 85/87 (98%)       | 76 (89%)    | 6 (7%)    | 3 (4%)    | 3           | 10  |
| 73  | o7    | 85/87 (98%)       | 72 (85%)    | 10 (12%)  | 3 (4%)    | 3           | 10  |
| 74  | O8    | 75/77 (97%)       | 62 (83%)    | 10 (13%)  | 3 (4%)    | 2           | 8   |
| 74  | o8    | 75/77 (97%)       | 66 (88%)    | 6 (8%)    | 3 (4%)    | 2           | 8   |
| 75  | O9    | 48/50 (96%)       | 44 (92%)    | 4 (8%)    | 0         | 100         | 100 |
| 75  | o9    | 48/50 (96%)       | 44 (92%)    | 3 (6%)    | 1 (2%)    | 5           | 20  |
| 76  | Q0    | 50/52 (96%)       | 48 (96%)    | 0         | 2 (4%)    | 2           | 8   |
| 76  | q0    | 50/52 (96%)       | 49 (98%)    | 0         | 1 (2%)    | 6           | 21  |
| 77  | Q1    | 23/25 (92%)       | 22 (96%)    | 1 (4%)    | 0         | 100         | 100 |
| 77  | q1    | 23/25 (92%)       | 23 (100%)   | 0         | 0         | 100         | 100 |
| 78  | Q2    | 103/105 (98%)     | 90 (87%)    | 10 (10%)  | 3 (3%)    | 3           | 13  |
| 78  | q2    | 103/105 (98%)     | 92 (89%)    | 8 (8%)    | 3 (3%)    | 3           | 13  |
| 79  | Q3    | 89/91 (98%)       | 80 (90%)    | 7 (8%)    | 2 (2%)    | 5           | 19  |
| 79  | q3    | 89/91 (98%)       | 80 (90%)    | 8 (9%)    | 1 (1%)    | 11          | 36  |
| 80  | e0    | 60/62 (97%)       | 47 (78%)    | 9 (15%)   | 4 (7%)    | 1           | 3   |
| 82  | p0    | 139/311 (45%)     | 117 (84%)   | 19 (14%)  | 3 (2%)    | 5           | 19  |
| All | All   | 22333/24141 (92%) | 19119 (86%) | 2092 (9%) | 1122 (5%) | 1           | 5   |

All (1122) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S0    | 39  | ASN  |
| 2   | S0    | 66  | ALA  |
| 2   | S0    | 103 | THR  |
| 2   | S0    | 158 | VAL  |
| 2   | S0    | 163 | ASN  |
| 2   | S0    | 191 | ARG  |
| 2   | S0    | 203 | PHE  |
| 3   | S1    | 49  | ASN  |
| 3   | S1    | 79  | HIS  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | S1    | 117 | TRP  |
| 3   | S1    | 132 | ASP  |
| 3   | S1    | 148 | ASN  |
| 3   | S1    | 179 | SER  |
| 3   | S1    | 206 | PRO  |
| 3   | S1    | 221 | PRO  |
| 4   | S2    | 148 | LEU  |
| 5   | S3    | 62  | ASN  |
| 5   | S3    | 64  | ARG  |
| 5   | S3    | 65  | ARG  |
| 5   | S3    | 93  | ASP  |
| 5   | S3    | 216 | PRO  |
| 5   | S3    | 220 | PRO  |
| 6   | S4    | 104 | ASP  |
| 6   | S4    | 164 | LEU  |
| 6   | S4    | 195 | ILE  |
| 6   | S4    | 223 | ASN  |
| 7   | S5    | 26  | ALA  |
| 7   | S5    | 35  | GLN  |
| 7   | S5    | 39  | GLU  |
| 7   | S5    | 43  | PHE  |
| 7   | S5    | 58  | LEU  |
| 7   | S5    | 60  | ASP  |
| 7   | S5    | 63  | GLN  |
| 7   | S5    | 101 | GLY  |
| 8   | S6    | 122 | GLU  |
| 8   | S6    | 173 | PRO  |
| 9   | S7    | 32  | PRO  |
| 9   | S7    | 64  | VAL  |
| 9   | S7    | 111 | LYS  |
| 9   | S7    | 112 | ARG  |
| 9   | S7    | 116 | ARG  |
| 9   | S7    | 131 | PHE  |
| 9   | S7    | 133 | THR  |
| 9   | S7    | 134 | GLU  |
| 9   | S7    | 155 | ASP  |
| 10  | S8    | 22  | ARG  |
| 10  | S8    | 152 | ILE  |
| 10  | S8    | 153 | GLU  |
| 11  | S9    | 98  | ALA  |
| 11  | S9    | 121 | SER  |
| 11  | S9    | 134 | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | S9    | 150 | LEU  |
| 12  | C0    | 60  | SER  |
| 12  | C0    | 87  | VAL  |
| 12  | C0    | 88  | PRO  |
| 13  | C1    | 7   | VAL  |
| 13  | C1    | 29  | LYS  |
| 14  | C2    | 25  | GLU  |
| 14  | C2    | 93  | ASP  |
| 14  | C2    | 101 | ALA  |
| 14  | C2    | 119 | SER  |
| 14  | C2    | 127 | GLY  |
| 15  | C3    | 22  | ALA  |
| 16  | C4    | 50  | ALA  |
| 16  | C4    | 124 | ASP  |
| 16  | C4    | 125 | SER  |
| 16  | C4    | 126 | THR  |
| 17  | C5    | 54  | ALA  |
| 17  | C5    | 125 | PRO  |
| 17  | C5    | 130 | ARG  |
| 18  | C6    | 39  | VAL  |
| 18  | C6    | 58  | ASP  |
| 18  | C6    | 97  | VAL  |
| 19  | C7    | 85  | VAL  |
| 19  | C7    | 86  | PRO  |
| 19  | C7    | 88  | VAL  |
| 19  | C7    | 124 | VAL  |
| 20  | C8    | 14  | ILE  |
| 20  | C8    | 61  | LEU  |
| 20  | C8    | 83  | ALA  |
| 20  | C8    | 91  | ASP  |
| 20  | C8    | 92  | ILE  |
| 21  | C9    | 53  | TRP  |
| 22  | D0    | 17  | GLN  |
| 24  | D2    | 83  | ILE  |
| 25  | D3    | 3   | LYS  |
| 25  | D3    | 92  | CYS  |
| 25  | D3    | 109 | ARG  |
| 25  | D3    | 144 | ARG  |
| 26  | D4    | 6   | THR  |
| 27  | D5    | 39  | ALA  |
| 27  | D5    | 43  | ASP  |
| 27  | D5    | 44  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | D5    | 71  | ILE  |
| 28  | D6    | 45  | VAL  |
| 28  | D6    | 82  | ARG  |
| 28  | D6    | 84  | VAL  |
| 28  | D6    | 85  | ARG  |
| 29  | D7    | 62  | ILE  |
| 31  | D9    | 8   | PHE  |
| 32  | E0    | 47  | VAL  |
| 33  | E1    | 102 | VAL  |
| 33  | E1    | 103 | LEU  |
| 33  | E1    | 106 | TYR  |
| 33  | E1    | 128 | ALA  |
| 33  | E1    | 138 | ARG  |
| 34  | SR    | 160 | GLU  |
| 35  | SM    | 52  | PRO  |
| 35  | SM    | 86  | ASN  |
| 35  | SM    | 87  | THR  |
| 35  | SM    | 102 | THR  |
| 35  | SM    | 140 | ASP  |
| 35  | SM    | 166 | VAL  |
| 35  | SM    | 167 | PRO  |
| 40  | L3    | 3   | HIS  |
| 40  | L3    | 4   | ARG  |
| 40  | L3    | 5   | LYS  |
| 40  | L3    | 139 | GLN  |
| 40  | L3    | 140 | ASP  |
| 40  | L3    | 174 | LYS  |
| 40  | L3    | 186 | GLY  |
| 41  | L4    | 4   | PRO  |
| 41  | L4    | 292 | SER  |
| 41  | L4    | 293 | SER  |
| 41  | L4    | 311 | HIS  |
| 41  | L4    | 317 | PRO  |
| 41  | L4    | 320 | ASN  |
| 42  | L5    | 57  | ASN  |
| 42  | L5    | 233 | ALA  |
| 42  | L5    | 234 | ASP  |
| 42  | L5    | 258 | LYS  |
| 43  | L6    | 6   | ALA  |
| 43  | L6    | 98  | VAL  |
| 44  | L7    | 26  | VAL  |
| 44  | L7    | 160 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | L8    | 25  | PRO  |
| 45  | L8    | 39  | ALA  |
| 46  | L9    | 190 | ASP  |
| 47  | M0    | 189 | GLU  |
| 47  | M0    | 219 | ALA  |
| 48  | M1    | 8   | PRO  |
| 48  | M1    | 9   | MET  |
| 48  | M1    | 11  | ASP  |
| 48  | M1    | 94  | ARG  |
| 48  | M1    | 115 | LYS  |
| 48  | M1    | 165 | GLN  |
| 49  | M3    | 47  | ALA  |
| 49  | M3    | 129 | ASN  |
| 49  | M3    | 134 | GLU  |
| 50  | M4    | 8   | LYS  |
| 50  | M4    | 9   | ALA  |
| 51  | M5    | 74  | PRO  |
| 51  | M5    | 144 | ARG  |
| 52  | M6    | 16  | VAL  |
| 52  | M6    | 111 | PRO  |
| 53  | M7    | 157 | VAL  |
| 53  | M7    | 182 | ILE  |
| 54  | M8    | 98  | LYS  |
| 54  | M8    | 99  | THR  |
| 56  | N0    | 2   | ALA  |
| 56  | N0    | 167 | ARG  |
| 57  | N1    | 124 | VAL  |
| 57  | N1    | 159 | PHE  |
| 58  | N2    | 31  | ALA  |
| 60  | N4    | 80  | ARG  |
| 60  | N4    | 81  | PRO  |
| 60  | N4    | 97  | LYS  |
| 62  | N6    | 52  | ARG  |
| 62  | N6    | 53  | ASP  |
| 62  | N6    | 84  | LYS  |
| 63  | N7    | 35  | SER  |
| 64  | N8    | 29  | PRO  |
| 64  | N8    | 76  | ASP  |
| 64  | N8    | 96  | LYS  |
| 67  | O1    | 5   | LYS  |
| 67  | O1    | 6   | ASP  |
| 67  | O1    | 84  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | O2    | 127 | ALA  |
| 71  | O5    | 119 | LYS  |
| 72  | O6    | 33  | ALA  |
| 72  | O6    | 34  | SER  |
| 74  | O8    | 33  | LYS  |
| 76  | Q0    | 78  | ILE  |
| 78  | Q2    | 15  | LYS  |
| 78  | Q2    | 100 | LYS  |
| 2   | s0    | 4   | PRO  |
| 2   | s0    | 44  | GLY  |
| 2   | s0    | 103 | THR  |
| 2   | s0    | 158 | VAL  |
| 2   | s0    | 164 | ASN  |
| 2   | s0    | 186 | GLY  |
| 2   | s0    | 189 | VAL  |
| 2   | s0    | 206 | ASP  |
| 3   | s1    | 62  | LYS  |
| 3   | s1    | 63  | GLY  |
| 3   | s1    | 81  | PHE  |
| 3   | s1    | 82  | ARG  |
| 3   | s1    | 147 | ALA  |
| 3   | s1    | 206 | PRO  |
| 3   | s1    | 223 | PHE  |
| 4   | s2    | 91  | ARG  |
| 4   | s2    | 92  | ALA  |
| 4   | s2    | 163 | GLY  |
| 5   | s3    | 61  | GLU  |
| 5   | s3    | 90  | ARG  |
| 5   | s3    | 115 | ILE  |
| 5   | s3    | 216 | PRO  |
| 5   | s3    | 217 | ILE  |
| 5   | s3    | 220 | PRO  |
| 6   | s4    | 104 | ASP  |
| 6   | s4    | 163 | ASP  |
| 6   | s4    | 164 | LEU  |
| 7   | s5    | 184 | PHE  |
| 8   | s6    | 153 | VAL  |
| 8   | s6    | 154 | ARG  |
| 8   | s6    | 173 | PRO  |
| 8   | s6    | 174 | LYS  |
| 9   | s7    | 10  | SER  |
| 9   | s7    | 64  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | s7    | 66  | SER  |
| 9   | s7    | 74  | GLN  |
| 9   | s7    | 116 | ARG  |
| 9   | s7    | 131 | PHE  |
| 9   | s7    | 163 | ASP  |
| 9   | s7    | 185 | ILE  |
| 10  | s8    | 115 | ALA  |
| 10  | s8    | 116 | HIS  |
| 12  | c0    | 32  | HIS  |
| 12  | c0    | 82  | LEU  |
| 12  | c0    | 83  | PRO  |
| 12  | c0    | 88  | PRO  |
| 12  | c0    | 92  | ILE  |
| 12  | c0    | 97  | PRO  |
| 13  | c1    | 114 | ALA  |
| 13  | c1    | 133 | LYS  |
| 13  | c1    | 144 | ALA  |
| 14  | c2    | 22  | VAL  |
| 14  | c2    | 89  | ILE  |
| 15  | c3    | 19  | SER  |
| 15  | c3    | 66  | ILE  |
| 15  | c3    | 87  | ASP  |
| 15  | c3    | 137 | PRO  |
| 15  | c3    | 139 | TRP  |
| 16  | c4    | 35  | GLY  |
| 16  | c4    | 126 | THR  |
| 16  | c4    | 132 | ARG  |
| 17  | c5    | 11  | VAL  |
| 17  | c5    | 51  | SER  |
| 17  | c5    | 52  | LYS  |
| 17  | c5    | 125 | PRO  |
| 17  | c5    | 126 | VAL  |
| 17  | c5    | 127 | ARG  |
| 18  | c6    | 42  | GLU  |
| 18  | c6    | 116 | LEU  |
| 19  | c7    | 67  | ARG  |
| 19  | c7    | 88  | VAL  |
| 19  | c7    | 99  | VAL  |
| 19  | c7    | 116 | LYS  |
| 20  | c8    | 92  | ILE  |
| 20  | c8    | 145 | ARG  |
| 21  | c9    | 28  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | c9    | 29  | GLU  |
| 21  | c9    | 33  | TYR  |
| 22  | d0    | 15  | GLN  |
| 22  | d0    | 49  | ASN  |
| 22  | d0    | 52  | LYS  |
| 26  | d4    | 30  | PRO  |
| 26  | d4    | 78  | SER  |
| 27  | d5    | 85  | LYS  |
| 27  | d5    | 104 | ALA  |
| 29  | d7    | 38  | PRO  |
| 29  | d7    | 60  | SER  |
| 29  | d7    | 62  | ILE  |
| 29  | d7    | 63  | LEU  |
| 30  | d8    | 33  | LEU  |
| 30  | d8    | 61  | ARG  |
| 31  | d9    | 6   | VAL  |
| 80  | e0    | 47  | VAL  |
| 80  | e0    | 60  | PRO  |
| 33  | e1    | 83  | LYS  |
| 33  | e1    | 87  | THR  |
| 33  | e1    | 92  | LYS  |
| 33  | e1    | 98  | VAL  |
| 33  | e1    | 103 | LEU  |
| 33  | e1    | 106 | TYR  |
| 34  | sR    | 4   | ASN  |
| 34  | sR    | 163 | ASP  |
| 34  | sR    | 165 | ASP  |
| 34  | sR    | 250 | TYR  |
| 35  | sM    | 47  | ALA  |
| 35  | sM    | 50  | ASN  |
| 35  | sM    | 64  | LYS  |
| 35  | sM    | 65  | THR  |
| 39  | l2    | 15  | ILE  |
| 40  | l3    | 3   | HIS  |
| 40  | l3    | 139 | GLN  |
| 40  | l3    | 293 | ASN  |
| 40  | l3    | 347 | SER  |
| 41  | l4    | 90  | PHE  |
| 41  | l4    | 272 | VAL  |
| 41  | l4    | 311 | HIS  |
| 41  | l4    | 329 | PRO  |
| 41  | l4    | 339 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | l5    | 260 | PHE  |
| 43  | l6    | 98  | VAL  |
| 45  | l8    | 25  | PRO  |
| 45  | l8    | 34  | PHE  |
| 45  | l8    | 117 | ALA  |
| 45  | l8    | 122 | LYS  |
| 46  | l9    | 144 | ILE  |
| 46  | l9    | 188 | THR  |
| 47  | m0    | 220 | GLN  |
| 48  | m1    | 8   | PRO  |
| 48  | m1    | 10  | ARG  |
| 48  | m1    | 94  | ARG  |
| 49  | m3    | 47  | ALA  |
| 49  | m3    | 51  | LEU  |
| 49  | m3    | 134 | GLU  |
| 51  | m5    | 48  | ALA  |
| 51  | m5    | 49  | ARG  |
| 51  | m5    | 76  | PRO  |
| 52  | m6    | 16  | VAL  |
| 52  | m6    | 110 | PRO  |
| 53  | m7    | 67  | ILE  |
| 54  | m8    | 98  | LYS  |
| 54  | m8    | 99  | THR  |
| 56  | n0    | 2   | ALA  |
| 57  | n1    | 122 | GLN  |
| 57  | n1    | 136 | ARG  |
| 60  | n4    | 76  | VAL  |
| 61  | n5    | 24  | LEU  |
| 61  | n5    | 25  | LYS  |
| 61  | n5    | 44  | PRO  |
| 61  | n5    | 45  | LYS  |
| 62  | n6    | 83  | ASP  |
| 62  | n6    | 84  | LYS  |
| 62  | n6    | 126 | LEU  |
| 63  | n7    | 5   | LEU  |
| 63  | n7    | 7   | ALA  |
| 63  | n7    | 125 | GLY  |
| 64  | n8    | 76  | ASP  |
| 65  | n9    | 21  | ILE  |
| 65  | n9    | 23  | LYS  |
| 65  | n9    | 39  | PHE  |
| 66  | o0    | 100 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67  | o1    | 83  | GLU  |
| 67  | o1    | 86  | LYS  |
| 69  | o3    | 88  | ASN  |
| 71  | o5    | 119 | LYS  |
| 72  | o6    | 33  | ALA  |
| 72  | o6    | 63  | ASN  |
| 72  | o6    | 98  | ARG  |
| 73  | o7    | 85  | LYS  |
| 74  | o8    | 18  | ALA  |
| 82  | p0    | 93  | LEU  |
| 2   | S0    | 5   | ALA  |
| 2   | S0    | 27  | ARG  |
| 2   | S0    | 30  | GLN  |
| 2   | S0    | 94  | GLY  |
| 2   | S0    | 95  | ALA  |
| 2   | S0    | 139 | VAL  |
| 2   | S0    | 185 | ARG  |
| 2   | S0    | 189 | VAL  |
| 2   | S0    | 192 | THR  |
| 2   | S0    | 194 | PRO  |
| 2   | S0    | 195 | TRP  |
| 3   | S1    | 35  | PRO  |
| 3   | S1    | 51  | SER  |
| 3   | S1    | 63  | GLY  |
| 3   | S1    | 93  | GLY  |
| 3   | S1    | 116 | LYS  |
| 3   | S1    | 213 | ARG  |
| 3   | S1    | 223 | PHE  |
| 4   | S2    | 145 | GLY  |
| 5   | S3    | 218 | LEU  |
| 6   | S4    | 12  | LEU  |
| 6   | S4    | 26  | CYS  |
| 6   | S4    | 222 | LEU  |
| 7   | S5    | 156 | ARG  |
| 7   | S5    | 204 | GLY  |
| 7   | S5    | 206 | SER  |
| 8   | S6    | 154 | ARG  |
| 8   | S6    | 174 | LYS  |
| 9   | S7    | 30  | SER  |
| 9   | S7    | 31  | SER  |
| 9   | S7    | 73  | VAL  |
| 9   | S7    | 85  | PHE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | S7    | 98  | ILE  |
| 9   | S7    | 156 | SER  |
| 10  | S8    | 59  | ARG  |
| 10  | S8    | 105 | ASP  |
| 10  | S8    | 120 | THR  |
| 11  | S9    | 169 | PRO  |
| 12  | C0    | 86  | ILE  |
| 13  | C1    | 4   | GLU  |
| 13  | C1    | 145 | ALA  |
| 13  | C1    | 154 | ALA  |
| 14  | C2    | 55  | GLY  |
| 14  | C2    | 91  | VAL  |
| 14  | C2    | 115 | VAL  |
| 14  | C2    | 125 | ASN  |
| 14  | C2    | 130 | THR  |
| 15  | C3    | 12  | SER  |
| 16  | C4    | 42  | VAL  |
| 16  | C4    | 51  | ASP  |
| 16  | C4    | 123 | SER  |
| 17  | C5    | 48  | GLY  |
| 17  | C5    | 101 | ALA  |
| 18  | C6    | 113 | ASP  |
| 20  | C8    | 7   | GLU  |
| 20  | C8    | 8   | GLN  |
| 20  | C8    | 82  | PRO  |
| 20  | C8    | 139 | LYS  |
| 21  | C9    | 69  | LYS  |
| 23  | D1    | 49  | GLU  |
| 25  | D3    | 8   | GLY  |
| 25  | D3    | 41  | SER  |
| 25  | D3    | 114 | LYS  |
| 25  | D3    | 131 | SER  |
| 26  | D4    | 4   | ALA  |
| 26  | D4    | 36  | SER  |
| 26  | D4    | 60  | PHE  |
| 28  | D6    | 18  | VAL  |
| 28  | D6    | 63  | ALA  |
| 28  | D6    | 86  | VAL  |
| 28  | D6    | 97  | PRO  |
| 29  | D7    | 60  | SER  |
| 29  | D7    | 75  | GLU  |
| 30  | D8    | 36  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | E1    | 84  | VAL  |
| 33  | E1    | 85  | TYR  |
| 33  | E1    | 98  | VAL  |
| 33  | E1    | 127 | GLY  |
| 34  | SR    | 98  | GLU  |
| 34  | SR    | 318 | ALA  |
| 35  | SM    | 82  | THR  |
| 35  | SM    | 88  | ARG  |
| 35  | SM    | 139 | GLU  |
| 39  | L2    | 250 | GLN  |
| 39  | L2    | 251 | LYS  |
| 40  | L3    | 351 | LEU  |
| 41  | L4    | 15  | ALA  |
| 41  | L4    | 190 | GLY  |
| 41  | L4    | 232 | SER  |
| 41  | L4    | 270 | SER  |
| 41  | L4    | 318 | LEU  |
| 41  | L4    | 339 | LEU  |
| 42  | L5    | 6   | ASP  |
| 42  | L5    | 137 | ASP  |
| 42  | L5    | 187 | THR  |
| 42  | L5    | 253 | PHE  |
| 42  | L5    | 260 | PHE  |
| 42  | L5    | 295 | GLY  |
| 44  | L7    | 24  | GLU  |
| 44  | L7    | 164 | SER  |
| 44  | L7    | 175 | LYS  |
| 45  | L8    | 157 | VAL  |
| 47  | M0    | 24  | ARG  |
| 47  | M0    | 194 | GLY  |
| 48  | M1    | 24  | GLY  |
| 48  | M1    | 167 | TYR  |
| 51  | M5    | 184 | LYS  |
| 52  | M6    | 182 | ASN  |
| 53  | M7    | 67  | ILE  |
| 53  | M7    | 160 | ALA  |
| 53  | M7    | 161 | ALA  |
| 58  | N2    | 11  | ILE  |
| 59  | N3    | 82  | ALA  |
| 60  | N4    | 64  | THR  |
| 62  | N6    | 126 | LEU  |
| 63  | N7    | 17  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | N7    | 18  | TYR  |
| 64  | N8    | 47  | LYS  |
| 64  | N8    | 66  | ALA  |
| 67  | O1    | 83  | GLU  |
| 70  | O4    | 77  | GLY  |
| 70  | O4    | 82  | ALA  |
| 71  | O5    | 90  | ARG  |
| 71  | O5    | 91  | ALA  |
| 72  | O6    | 28  | TYR  |
| 73  | O7    | 79  | GLN  |
| 78  | Q2    | 94  | GLY  |
| 79  | Q3    | 51  | ALA  |
| 2   | s0    | 30  | GLN  |
| 2   | s0    | 94  | GLY  |
| 2   | s0    | 95  | ALA  |
| 2   | s0    | 185 | ARG  |
| 3   | s1    | 93  | GLY  |
| 4   | s2    | 107 | SER  |
| 4   | s2    | 164 | SER  |
| 4   | s2    | 228 | ASN  |
| 6   | s4    | 12  | LEU  |
| 6   | s4    | 24  | SER  |
| 6   | s4    | 195 | ILE  |
| 6   | s4    | 196 | VAL  |
| 7   | s5    | 28  | PRO  |
| 7   | s5    | 36  | ALA  |
| 7   | s5    | 43  | PHE  |
| 7   | s5    | 54  | LYS  |
| 7   | s5    | 151 | GLY  |
| 8   | s6    | 68  | LEU  |
| 8   | s6    | 122 | GLU  |
| 10  | s8    | 62  | THR  |
| 10  | s8    | 101 | ILE  |
| 11  | s9    | 110 | GLN  |
| 11  | s9    | 134 | ILE  |
| 11  | s9    | 183 | ALA  |
| 12  | c0    | 23  | ALA  |
| 12  | c0    | 31  | LYS  |
| 12  | c0    | 35  | ILE  |
| 13  | c1    | 55  | ASP  |
| 14  | c2    | 58  | LEU  |
| 14  | c2    | 101 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | c2    | 119 | SER  |
| 14  | c2    | 131 | ASP  |
| 15  | c3    | 140 | LYS  |
| 16  | c4    | 50  | ALA  |
| 16  | c4    | 51  | ASP  |
| 16  | c4    | 124 | ASP  |
| 16  | c4    | 131 | GLY  |
| 17  | c5    | 17  | TYR  |
| 17  | c5    | 132 | GLY  |
| 19  | c7    | 113 | LEU  |
| 20  | c8    | 61  | LEU  |
| 20  | c8    | 135 | GLY  |
| 22  | d0    | 17  | GLN  |
| 23  | d1    | 4   | ASP  |
| 23  | d1    | 77  | GLY  |
| 25  | d3    | 131 | SER  |
| 26  | d4    | 33  | ALA  |
| 26  | d4    | 35  | VAL  |
| 26  | d4    | 53  | ASP  |
| 27  | d5    | 38  | HIS  |
| 27  | d5    | 83  | LEU  |
| 28  | d6    | 62  | TYR  |
| 29  | d7    | 20  | LYS  |
| 29  | d7    | 50  | ALA  |
| 29  | d7    | 75  | GLU  |
| 31  | d9    | 7   | TRP  |
| 31  | d9    | 19  | ARG  |
| 80  | e0    | 61  | SER  |
| 33  | e1    | 84  | VAL  |
| 33  | e1    | 97  | LYS  |
| 33  | e1    | 102 | VAL  |
| 33  | e1    | 127 | GLY  |
| 39  | l2    | 215 | ASN  |
| 39  | l2    | 238 | ILE  |
| 39  | l2    | 249 | SER  |
| 40  | l3    | 138 | ALA  |
| 41  | l4    | 302 | ALA  |
| 42  | l5    | 135 | VAL  |
| 42  | l5    | 258 | LYS  |
| 42  | l5    | 270 | LYS  |
| 43  | l6    | 97  | ASN  |
| 45  | l8    | 39  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | l8    | 79  | GLN  |
| 45  | l8    | 114 | ALA  |
| 45  | l8    | 121 | SER  |
| 45  | l8    | 188 | THR  |
| 45  | l8    | 190 | VAL  |
| 45  | l8    | 203 | VAL  |
| 47  | m0    | 204 | GLY  |
| 47  | m0    | 207 | GLU  |
| 48  | m1    | 7   | ASN  |
| 49  | m3    | 129 | ASN  |
| 49  | m3    | 141 | ALA  |
| 50  | m4    | 3   | THR  |
| 50  | m4    | 135 | LEU  |
| 51  | m5    | 183 | THR  |
| 51  | m5    | 184 | LYS  |
| 54  | m8    | 41  | ASP  |
| 54  | m8    | 167 | SER  |
| 54  | m8    | 171 | LYS  |
| 55  | m9    | 35  | ALA  |
| 55  | m9    | 155 | LEU  |
| 55  | m9    | 156 | ASN  |
| 56  | n0    | 50  | LYS  |
| 57  | n1    | 127 | GLN  |
| 58  | n2    | 51  | GLY  |
| 60  | n4    | 63  | ILE  |
| 60  | n4    | 71  | ARG  |
| 60  | n4    | 77  | LYS  |
| 62  | n6    | 92  | GLY  |
| 62  | n6    | 125 | LYS  |
| 63  | n7    | 16  | GLY  |
| 64  | n8    | 47  | LYS  |
| 64  | n8    | 129 | PHE  |
| 67  | o1    | 84  | ASP  |
| 68  | o2    | 124 | GLY  |
| 70  | o4    | 77  | GLY  |
| 72  | o6    | 12  | ASN  |
| 72  | o6    | 64  | SER  |
| 74  | o8    | 15  | THR  |
| 82  | p0    | 47  | GLY  |
| 3   | S1    | 26  | ARG  |
| 3   | S1    | 58  | SER  |
| 3   | S1    | 78  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | S1    | 147 | ALA  |
| 4   | S2    | 79  | GLU  |
| 4   | S2    | 91  | ARG  |
| 4   | S2    | 107 | SER  |
| 4   | S2    | 235 | LEU  |
| 4   | S2    | 248 | SER  |
| 6   | S4    | 77  | ARG  |
| 6   | S4    | 245 | LYS  |
| 7   | S5    | 127 | GLN  |
| 7   | S5    | 150 | GLY  |
| 8   | S6    | 70  | PRO  |
| 8   | S6    | 152 | ASP  |
| 9   | S7    | 84  | LYS  |
| 10  | S8    | 9   | HIS  |
| 10  | S8    | 40  | ALA  |
| 10  | S8    | 149 | SER  |
| 10  | S8    | 199 | LYS  |
| 11  | S9    | 118 | LEU  |
| 11  | S9    | 164 | PHE  |
| 12  | C0    | 94  | GLU  |
| 13  | C1    | 3   | THR  |
| 13  | C1    | 55  | ASP  |
| 13  | C1    | 153 | PHE  |
| 14  | C2    | 21  | GLU  |
| 14  | C2    | 22  | VAL  |
| 14  | C2    | 39  | ASP  |
| 16  | C4    | 40  | ALA  |
| 16  | C4    | 75  | GLY  |
| 17  | C5    | 51  | SER  |
| 17  | C5    | 69  | GLU  |
| 17  | C5    | 126 | VAL  |
| 19  | C7    | 120 | SER  |
| 20  | C8    | 60  | GLU  |
| 25  | D3    | 112 | LYS  |
| 26  | D4    | 34  | ASN  |
| 26  | D4    | 58  | PHE  |
| 26  | D4    | 133 | ASN  |
| 28  | D6    | 10  | ARG  |
| 28  | D6    | 62  | TYR  |
| 28  | D6    | 65  | PRO  |
| 29  | D7    | 38  | PRO  |
| 33  | E1    | 83  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | E1    | 86  | THR  |
| 33  | E1    | 87  | THR  |
| 33  | E1    | 118 | ARG  |
| 34  | SR    | 50  | ASP  |
| 34  | SR    | 161 | LYS  |
| 34  | SR    | 228 | LYS  |
| 35  | SM    | 53  | ARG  |
| 35  | SM    | 89  | ARG  |
| 35  | SM    | 153 | ASP  |
| 35  | SM    | 174 | LEU  |
| 40  | L3    | 155 | ALA  |
| 40  | L3    | 300 | ARG  |
| 41  | L4    | 5   | GLN  |
| 41  | L4    | 16  | THR  |
| 42  | L5    | 58  | LYS  |
| 42  | L5    | 188 | GLU  |
| 42  | L5    | 252 | ALA  |
| 42  | L5    | 259 | LYS  |
| 44  | L7    | 25  | GLN  |
| 44  | L7    | 212 | GLY  |
| 45  | L8    | 117 | ALA  |
| 45  | L8    | 255 | SER  |
| 46  | L9    | 2   | LYS  |
| 47  | M0    | 211 | ARG  |
| 48  | M1    | 7   | ASN  |
| 49  | M3    | 76  | THR  |
| 49  | M3    | 130 | GLY  |
| 49  | M3    | 131 | LYS  |
| 50  | M4    | 28  | SER  |
| 50  | M4    | 136 | ALA  |
| 53  | M7    | 164 | LYS  |
| 54  | M8    | 183 | GLY  |
| 57  | N1    | 125 | ALA  |
| 58  | N2    | 91  | ASP  |
| 63  | N7    | 33  | SER  |
| 63  | N7    | 78  | ASN  |
| 65  | N9    | 57  | ALA  |
| 72  | O6    | 3   | VAL  |
| 72  | O6    | 21  | THR  |
| 72  | O6    | 95  | ALA  |
| 72  | O6    | 98  | ARG  |
| 73  | O7    | 85  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | s0    | 68  | PRO  |
| 2   | s0    | 102 | PHE  |
| 3   | s1    | 26  | ARG  |
| 3   | s1    | 154 | SER  |
| 4   | s2    | 238 | SER  |
| 5   | s3    | 93  | ASP  |
| 6   | s4    | 57  | ASN  |
| 6   | s4    | 245 | LYS  |
| 7   | s5    | 100 | ASN  |
| 7   | s5    | 127 | GLN  |
| 7   | s5    | 153 | GLY  |
| 10  | s8    | 199 | LYS  |
| 11  | s9    | 5   | PRO  |
| 11  | s9    | 105 | LEU  |
| 11  | s9    | 147 | MET  |
| 12  | c0    | 30  | ALA  |
| 13  | c1    | 61  | THR  |
| 13  | c1    | 132 | SER  |
| 13  | c1    | 146 | ALA  |
| 14  | c2    | 26  | ASP  |
| 14  | c2    | 59  | LEU  |
| 14  | c2    | 87  | PRO  |
| 14  | c2    | 103 | LEU  |
| 14  | c2    | 106 | ILE  |
| 14  | c2    | 107 | ASP  |
| 14  | c2    | 108 | ARG  |
| 14  | c2    | 118 | ALA  |
| 16  | c4    | 12  | GLN  |
| 16  | c4    | 92  | LYS  |
| 17  | c5    | 8   | LYS  |
| 17  | c5    | 49  | MET  |
| 17  | c5    | 68  | PRO  |
| 17  | c5    | 80  | MET  |
| 17  | c5    | 128 | HIS  |
| 17  | c5    | 129 | GLY  |
| 18  | c6    | 39  | VAL  |
| 18  | c6    | 97  | VAL  |
| 18  | c6    | 142 | TYR  |
| 19  | c7    | 120 | SER  |
| 20  | c8    | 91  | ASP  |
| 23  | d1    | 44  | ARG  |
| 23  | d1    | 78  | LEU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | d2    | 68  | ARG  |
| 26  | d4    | 51  | GLU  |
| 26  | d4    | 58  | PHE  |
| 28  | d6    | 46  | GLU  |
| 28  | d6    | 63  | ALA  |
| 29  | d7    | 3   | LEU  |
| 30  | d8    | 62  | GLU  |
| 80  | e0    | 54  | ARG  |
| 33  | e1    | 81  | LYS  |
| 33  | e1    | 110 | ALA  |
| 33  | e1    | 128 | ALA  |
| 33  | e1    | 148 | TYR  |
| 34  | sR    | 146 | GLY  |
| 34  | sR    | 161 | LYS  |
| 35  | sM    | 48  | ARG  |
| 35  | sM    | 66  | ALA  |
| 35  | sM    | 78  | ASP  |
| 35  | sM    | 167 | PRO  |
| 39  | l2    | 96  | LEU  |
| 39  | l2    | 142 | ASP  |
| 41  | l4    | 145 | ILE  |
| 43  | l6    | 32  | ALA  |
| 45  | l8    | 26  | LEU  |
| 45  | l8    | 120 | LYS  |
| 45  | l8    | 123 | GLN  |
| 45  | l8    | 124 | ASP  |
| 45  | l8    | 133 | LYS  |
| 45  | l8    | 237 | ILE  |
| 46  | l9    | 107 | ASP  |
| 47  | m0    | 3   | ARG  |
| 47  | m0    | 195 | ALA  |
| 47  | m0    | 219 | ALA  |
| 48  | m1    | 95  | ASN  |
| 48  | m1    | 173 | ASP  |
| 49  | m3    | 19  | GLN  |
| 49  | m3    | 135 | ALA  |
| 53  | m7    | 66  | SER  |
| 54  | m8    | 91  | ALA  |
| 56  | n0    | 138 | GLN  |
| 57  | n1    | 135 | PRO  |
| 60  | n4    | 83  | THR  |
| 60  | n4    | 127 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | n5    | 47  | ALA  |
| 63  | n7    | 127 | ASN  |
| 64  | n8    | 78  | LEU  |
| 68  | o2    | 6   | HIS  |
| 69  | o3    | 91  | ALA  |
| 69  | o3    | 92  | LYS  |
| 70  | o4    | 82  | ALA  |
| 71  | o5    | 40  | SER  |
| 72  | o6    | 34  | SER  |
| 73  | o7    | 86  | ALA  |
| 74  | o8    | 17  | ARG  |
| 75  | o9    | 3   | ALA  |
| 76  | q0    | 78  | ILE  |
| 2   | S0    | 4   | PRO  |
| 2   | S0    | 36  | TYR  |
| 3   | S1    | 54  | LEU  |
| 3   | S1    | 55  | LYS  |
| 3   | S1    | 82  | ARG  |
| 3   | S1    | 158 | SER  |
| 3   | S1    | 209 | ASN  |
| 4   | S2    | 150 | GLN  |
| 5   | S3    | 217 | ILE  |
| 6   | S4    | 157 | ASN  |
| 6   | S4    | 193 | GLY  |
| 7   | S5    | 21  | THR  |
| 7   | S5    | 45  | LYS  |
| 7   | S5    | 64  | VAL  |
| 7   | S5    | 79  | ASN  |
| 7   | S5    | 154 | ALA  |
| 8   | S6    | 165 | GLY  |
| 10  | S8    | 10  | LYS  |
| 10  | S8    | 52  | ASN  |
| 12  | C0    | 34  | GLU  |
| 14  | C2    | 89  | ILE  |
| 14  | C2    | 106 | ILE  |
| 14  | C2    | 107 | ASP  |
| 14  | C2    | 108 | ARG  |
| 14  | C2    | 112 | ALA  |
| 14  | C2    | 131 | ASP  |
| 15  | C3    | 106 | ARG  |
| 16  | C4    | 18  | ARG  |
| 16  | C4    | 86  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | C4    | 114 | ARG  |
| 17  | C5    | 24  | LYS  |
| 17  | C5    | 52  | LYS  |
| 18  | C6    | 41  | PRO  |
| 21  | C9    | 29  | GLU  |
| 21  | C9    | 130 | ARG  |
| 23  | D1    | 10  | GLU  |
| 23  | D1    | 28  | ASP  |
| 23  | D1    | 81  | ASN  |
| 25  | D3    | 40  | SER  |
| 26  | D4    | 5   | VAL  |
| 27  | D5    | 41  | ILE  |
| 28  | D6    | 36  | ILE  |
| 28  | D6    | 64  | LEU  |
| 29  | D7    | 63  | LEU  |
| 30  | D8    | 61  | ARG  |
| 31  | D9    | 34  | TYR  |
| 33  | E1    | 94  | LYS  |
| 33  | E1    | 100 | LEU  |
| 33  | E1    | 137 | ASP  |
| 33  | E1    | 148 | TYR  |
| 34  | SR    | 51  | ASP  |
| 34  | SR    | 117 | LYS  |
| 34  | SR    | 163 | ASP  |
| 34  | SR    | 237 | GLN  |
| 35  | SM    | 97  | THR  |
| 35  | SM    | 172 | VAL  |
| 35  | SM    | 173 | GLU  |
| 40  | L3    | 385 | LYS  |
| 41  | L4    | 182 | LEU  |
| 41  | L4    | 233 | LEU  |
| 42  | L5    | 7   | ALA  |
| 42  | L5    | 115 | LEU  |
| 42  | L5    | 125 | VAL  |
| 43  | L6    | 5   | LYS  |
| 45  | L8    | 120 | LYS  |
| 46  | L9    | 66  | ALA  |
| 46  | L9    | 189 | GLU  |
| 48  | M1    | 64  | LYS  |
| 48  | M1    | 114 | ILE  |
| 49  | M3    | 136 | GLU  |
| 51  | M5    | 75  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | M8    | 162 | ALA  |
| 55  | M9    | 53  | LYS  |
| 60  | N4    | 76  | VAL  |
| 64  | N8    | 94  | ALA  |
| 73  | O7    | 86  | ALA  |
| 4   | s2    | 235 | LEU  |
| 6   | s4    | 90  | ILE  |
| 7   | s5    | 29  | ILE  |
| 7   | s5    | 39  | GLU  |
| 7   | s5    | 60  | ASP  |
| 7   | s5    | 125 | THR  |
| 9   | s7    | 11  | GLN  |
| 9   | s7    | 133 | THR  |
| 10  | s8    | 52  | ASN  |
| 11  | s9    | 3   | ARG  |
| 11  | s9    | 65  | LYS  |
| 11  | s9    | 168 | ARG  |
| 14  | c2    | 54  | ARG  |
| 14  | c2    | 115 | VAL  |
| 15  | c3    | 29  | SER  |
| 15  | c3    | 60  | VAL  |
| 16  | c4    | 114 | ARG  |
| 17  | c5    | 14  | THR  |
| 17  | c5    | 69  | GLU  |
| 17  | c5    | 130 | ARG  |
| 18  | c6    | 115 | THR  |
| 20  | c8    | 60  | GLU  |
| 22  | d0    | 51  | VAL  |
| 22  | d0    | 118 | VAL  |
| 23  | d1    | 21  | ASN  |
| 27  | d5    | 53  | GLU  |
| 28  | d6    | 11  | ASN  |
| 28  | d6    | 59  | TYR  |
| 29  | d7    | 59  | CYS  |
| 33  | e1    | 100 | LEU  |
| 33  | e1    | 131 | PHE  |
| 33  | e1    | 144 | CYS  |
| 34  | sR    | 149 | ASP  |
| 34  | sR    | 317 | THR  |
| 35  | sM    | 63  | ASP  |
| 35  | sM    | 120 | GLU  |
| 39  | l2    | 24  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | l2    | 56  | ALA  |
| 40  | l3    | 155 | ALA  |
| 40  | l3    | 333 | LYS  |
| 41  | l4    | 305 | ALA  |
| 41  | l4    | 330 | TYR  |
| 42  | l5    | 44  | TYR  |
| 42  | l5    | 158 | ARG  |
| 43  | l6    | 10  | TYR  |
| 44  | l7    | 191 | VAL  |
| 45  | l8    | 240 | ASN  |
| 46  | l9    | 62  | ARG  |
| 46  | l9    | 167 | VAL  |
| 48  | m1    | 117 | ASP  |
| 48  | m1    | 167 | TYR  |
| 49  | m3    | 93  | ILE  |
| 49  | m3    | 101 | ARG  |
| 53  | m7    | 75  | GLU  |
| 58  | n2    | 49  | ASN  |
| 58  | n2    | 50  | LEU  |
| 59  | n3    | 46  | LEU  |
| 60  | n4    | 72  | SER  |
| 60  | n4    | 132 | GLY  |
| 63  | n7    | 103 | GLN  |
| 68  | o2    | 5   | PRO  |
| 73  | o7    | 84  | SER  |
| 78  | q2    | 32  | LYS  |
| 2   | S0    | 81  | PHE  |
| 2   | S0    | 164 | ASN  |
| 2   | S0    | 205 | ARG  |
| 3   | S1    | 81  | PHE  |
| 5   | S3    | 196 | ARG  |
| 7   | S5    | 51  | VAL  |
| 7   | S5    | 65  | ARG  |
| 11  | S9    | 99  | LEU  |
| 11  | S9    | 163 | PRO  |
| 14  | C2    | 66  | VAL  |
| 14  | C2    | 87  | PRO  |
| 14  | C2    | 129 | GLU  |
| 17  | C5    | 22  | LEU  |
| 19  | C7    | 115 | LEU  |
| 20  | C8    | 144 | ARG  |
| 22  | D0    | 21  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | D1    | 12  | TYR  |
| 27  | D5    | 38  | HIS  |
| 27  | D5    | 42  | LEU  |
| 33  | E1    | 93  | HIS  |
| 35  | SM    | 12  | VAL  |
| 35  | SM    | 64  | LYS  |
| 39  | L2    | 143 | GLU  |
| 40  | L3    | 317 | ILE  |
| 41  | L4    | 14  | GLU  |
| 41  | L4    | 130 | ALA  |
| 44  | L7    | 158 | LYS  |
| 45  | L8    | 36  | ILE  |
| 45  | L8    | 78  | PHE  |
| 48  | M1    | 151 | SER  |
| 49  | M3    | 153 | ASP  |
| 50  | M4    | 6   | ILE  |
| 57  | N1    | 18  | ASP  |
| 57  | N1    | 123 | GLY  |
| 58  | N2    | 10  | LYS  |
| 61  | N5    | 50  | ALA  |
| 63  | N7    | 36  | HIS  |
| 63  | N7    | 102 | GLU  |
| 63  | N7    | 103 | GLN  |
| 64  | N8    | 117 | ARG  |
| 66  | O0    | 71  | GLN  |
| 67  | O1    | 7   | VAL  |
| 69  | O3    | 59  | VAL  |
| 70  | O4    | 3   | GLN  |
| 71  | O5    | 75  | TYR  |
| 76  | Q0    | 79  | GLU  |
| 79  | Q3    | 7   | LYS  |
| 2   | s0    | 10  | THR  |
| 4   | s2    | 106 | ASP  |
| 4   | s2    | 150 | GLN  |
| 5   | s3    | 145 | ALA  |
| 5   | s3    | 179 | GLN  |
| 5   | s3    | 196 | ARG  |
| 5   | s3    | 219 | ALA  |
| 7   | s5    | 71  | ALA  |
| 9   | s7    | 67  | LEU  |
| 10  | s8    | 136 | SER  |
| 10  | s8    | 148 | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | s9    | 91  | LYS  |
| 11  | s9    | 146 | PHE  |
| 12  | c0    | 24  | LYS  |
| 12  | c0    | 95  | ARG  |
| 13  | c1    | 129 | ARG  |
| 14  | c2    | 82  | PRO  |
| 14  | c2    | 92  | ALA  |
| 15  | c3    | 22  | ALA  |
| 17  | c5    | 6   | ASN  |
| 17  | c5    | 131 | ALA  |
| 18  | c6    | 40  | GLU  |
| 26  | d4    | 34  | ASN  |
| 26  | d4    | 50  | ALA  |
| 28  | d6    | 8   | ASN  |
| 28  | d6    | 35  | ALA  |
| 28  | d6    | 60  | PRO  |
| 30  | d8    | 64  | ARG  |
| 31  | d9    | 11  | PRO  |
| 35  | sM    | 43  | ASP  |
| 35  | sM    | 83  | LYS  |
| 39  | l2    | 247 | ARG  |
| 40  | l3    | 37  | ARG  |
| 40  | l3    | 187 | SER  |
| 41  | l4    | 5   | GLN  |
| 41  | l4    | 146 | PRO  |
| 41  | l4    | 233 | LEU  |
| 42  | l5    | 125 | VAL  |
| 42  | l5    | 216 | GLU  |
| 44  | l7    | 229 | PHE  |
| 45  | l8    | 81  | THR  |
| 45  | l8    | 115 | ALA  |
| 47  | m0    | 193 | ASP  |
| 48  | m1    | 114 | ILE  |
| 48  | m1    | 115 | LYS  |
| 49  | m3    | 50  | PRO  |
| 49  | m3    | 76  | THR  |
| 51  | m5    | 68  | ARG  |
| 51  | m5    | 81  | TYR  |
| 63  | n7    | 28  | PRO  |
| 63  | n7    | 134 | LEU  |
| 65  | n9    | 25  | LYS  |
| 78  | q2    | 33  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | p0    | 33  | VAL  |
| 3   | S1    | 210 | ILE  |
| 4   | S2    | 106 | ASP  |
| 6   | S4    | 233 | LYS  |
| 8   | S6    | 146 | GLY  |
| 9   | S7    | 36  | ALA  |
| 10  | S8    | 147 | ALA  |
| 13  | C1    | 5   | LEU  |
| 13  | C1    | 6   | THR  |
| 14  | C2    | 126 | TRP  |
| 19  | C7    | 24  | LEU  |
| 21  | C9    | 35  | ASP  |
| 27  | D5    | 88  | ILE  |
| 28  | D6    | 59  | TYR  |
| 30  | D8    | 34  | GLU  |
| 33  | E1    | 111 | GLU  |
| 34  | SR    | 105 | GLY  |
| 39  | L2    | 13  | GLY  |
| 40  | L3    | 299 | ASP  |
| 42  | L5    | 221 | GLU  |
| 44  | L7    | 178 | ILE  |
| 48  | M1    | 117 | ASP  |
| 48  | M1    | 138 | VAL  |
| 51  | M5    | 94  | TYR  |
| 63  | N7    | 125 | GLY  |
| 64  | N8    | 97  | GLU  |
| 65  | N9    | 21  | ILE  |
| 72  | O6    | 78  | GLY  |
| 74  | O8    | 35  | GLY  |
| 2   | s0    | 139 | VAL  |
| 3   | s1    | 21  | VAL  |
| 3   | s1    | 22  | ASP  |
| 5   | s3    | 180 | GLY  |
| 6   | s4    | 30  | ARG  |
| 6   | s4    | 168 | LYS  |
| 7   | s5    | 21  | THR  |
| 7   | s5    | 59  | VAL  |
| 10  | s8    | 78  | ILE  |
| 11  | s9    | 126 | ARG  |
| 12  | c0    | 3   | MET  |
| 14  | c2    | 25  | GLU  |
| 14  | c2    | 66  | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | c9    | 66  | TYR  |
| 26  | d4    | 52  | LYS  |
| 27  | d5    | 87  | GLY  |
| 30  | d8    | 32  | PHE  |
| 33  | e1    | 145 | HIS  |
| 41  | l4    | 328 | ASN  |
| 42  | l5    | 215 | ASP  |
| 69  | o3    | 59  | VAL  |
| 72  | o6    | 3   | VAL  |
| 78  | q2    | 31  | GLY  |
| 79  | q3    | 51  | ALA  |
| 9   | S7    | 13  | PRO  |
| 14  | C2    | 117 | GLY  |
| 34  | SR    | 15  | GLY  |
| 34  | SR    | 188 | ILE  |
| 63  | N7    | 16  | GLY  |
| 4   | s2    | 93  | GLY  |
| 7   | s5    | 33  | VAL  |
| 9   | s7    | 13  | PRO  |
| 22  | d0    | 96  | PRO  |
| 26  | d4    | 129 | VAL  |
| 33  | e1    | 124 | PRO  |
| 47  | m0    | 117 | GLY  |
| 66  | o0    | 10  | ILE  |
| 14  | C2    | 40  | GLY  |
| 41  | L4    | 328 | ASN  |
| 4   | s2    | 83  | ILE  |
| 8   | s6    | 69  | LEU  |
| 8   | s6    | 70  | PRO  |
| 9   | s7    | 32  | PRO  |
| 13  | c1    | 7   | VAL  |
| 69  | o3    | 61  | GLY  |
| 3   | S1    | 48  | VAL  |
| 7   | S5    | 153 | GLY  |
| 14  | C2    | 81  | ASP  |
| 23  | D1    | 6   | GLY  |
| 41  | L4    | 131 | VAL  |
| 41  | L4    | 146 | PRO  |
| 46  | L9    | 13  | PRO  |
| 66  | O0    | 100 | ILE  |
| 74  | O8    | 37  | PRO  |
| 9   | s7    | 73  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | c6    | 4   | VAL  |
| 20  | c8    | 14  | ILE  |
| 21  | c9    | 3   | GLY  |
| 22  | d0    | 97  | VAL  |
| 33  | e1    | 112 | GLY  |
| 44  | l7    | 178 | ILE  |
| 3   | S1    | 21  | VAL  |
| 25  | D3    | 108 | GLY  |
| 31  | D9    | 6   | VAL  |
| 35  | SM    | 17  | VAL  |
| 51  | M5    | 89  | VAL  |
| 52  | M6    | 110 | PRO  |
| 5   | s3    | 203 | PRO  |
| 14  | c2    | 91  | VAL  |
| 14  | c2    | 121 | VAL  |
| 17  | c5    | 48  | GLY  |
| 35  | sM    | 172 | VAL  |
| 67  | o1    | 45  | GLY  |
| 3   | S1    | 22  | ASP  |
| 46  | l9    | 187 | ILE  |
| 54  | m8    | 84  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 2   | S0    | 164/209 (78%) | 131 (80%) | 33 (20%) | 1           | 4 |
| 2   | s0    | 165/209 (79%) | 129 (78%) | 36 (22%) | 1           | 3 |
| 3   | S1    | 191/223 (86%) | 161 (84%) | 30 (16%) | 2           | 9 |
| 3   | s1    | 192/223 (86%) | 155 (81%) | 37 (19%) | 1           | 5 |
| 4   | S2    | 176/204 (86%) | 130 (74%) | 46 (26%) | 0           | 2 |
| 4   | s2    | 176/204 (86%) | 136 (77%) | 40 (23%) | 1           | 3 |
| 5   | S3    | 182/194 (94%) | 145 (80%) | 37 (20%) | 1           | 4 |
| 5   | s3    | 182/194 (94%) | 145 (80%) | 37 (20%) | 1           | 4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | S4    | 221/221 (100%) | 175 (79%) | 46 (21%) | 1           | 4  |
| 6   | s4    | 221/221 (100%) | 181 (82%) | 40 (18%) | 2           | 6  |
| 7   | S5    | 173/190 (91%)  | 144 (83%) | 29 (17%) | 2           | 8  |
| 7   | s5    | 173/190 (91%)  | 134 (78%) | 39 (22%) | 1           | 3  |
| 8   | S6    | 188/201 (94%)  | 149 (79%) | 39 (21%) | 1           | 4  |
| 8   | s6    | 187/201 (93%)  | 150 (80%) | 37 (20%) | 1           | 5  |
| 9   | S7    | 165/169 (98%)  | 132 (80%) | 33 (20%) | 1           | 4  |
| 9   | s7    | 165/169 (98%)  | 127 (77%) | 38 (23%) | 1           | 3  |
| 10  | S8    | 150/161 (93%)  | 127 (85%) | 23 (15%) | 3           | 10 |
| 10  | s8    | 150/161 (93%)  | 127 (85%) | 23 (15%) | 3           | 10 |
| 11  | S9    | 158/165 (96%)  | 121 (77%) | 37 (23%) | 1           | 3  |
| 11  | s9    | 158/165 (96%)  | 127 (80%) | 31 (20%) | 1           | 5  |
| 12  | C0    | 77/98 (79%)    | 59 (77%)  | 18 (23%) | 1           | 3  |
| 12  | c0    | 73/98 (74%)    | 59 (81%)  | 14 (19%) | 1           | 5  |
| 13  | C1    | 129/136 (95%)  | 102 (79%) | 27 (21%) | 1           | 4  |
| 13  | c1    | 129/136 (95%)  | 105 (81%) | 24 (19%) | 1           | 5  |
| 14  | C2    | 88/118 (75%)   | 66 (75%)  | 22 (25%) | 0           | 2  |
| 14  | c2    | 88/118 (75%)   | 63 (72%)  | 25 (28%) | 0           | 1  |
| 15  | C3    | 127/127 (100%) | 100 (79%) | 27 (21%) | 1           | 4  |
| 15  | c3    | 127/127 (100%) | 102 (80%) | 25 (20%) | 1           | 5  |
| 16  | C4    | 81/104 (78%)   | 61 (75%)  | 20 (25%) | 1           | 2  |
| 16  | c4    | 97/104 (93%)   | 77 (79%)  | 20 (21%) | 1           | 4  |
| 17  | C5    | 101/117 (86%)  | 84 (83%)  | 17 (17%) | 2           | 8  |
| 17  | c5    | 103/117 (88%)  | 82 (80%)  | 21 (20%) | 1           | 4  |
| 18  | C6    | 117/118 (99%)  | 94 (80%)  | 23 (20%) | 1           | 5  |
| 18  | c6    | 118/118 (100%) | 96 (81%)  | 22 (19%) | 1           | 5  |
| 19  | C7    | 94/124 (76%)   | 72 (77%)  | 22 (23%) | 1           | 3  |
| 19  | c7    | 92/124 (74%)   | 74 (80%)  | 18 (20%) | 1           | 5  |
| 20  | C8    | 128/128 (100%) | 99 (77%)  | 29 (23%) | 1           | 3  |
| 20  | c8    | 128/128 (100%) | 98 (77%)  | 30 (23%) | 1           | 3  |
| 21  | C9    | 115/115 (100%) | 92 (80%)  | 23 (20%) | 1           | 4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 21  | c9    | 115/115 (100%) | 91 (79%)  | 24 (21%) | 1           | 4  |
| 22  | D0    | 100/113 (88%)  | 68 (68%)  | 32 (32%) | 0           | 1  |
| 22  | d0    | 103/113 (91%)  | 77 (75%)  | 26 (25%) | 0           | 2  |
| 23  | D1    | 74/74 (100%)   | 59 (80%)  | 15 (20%) | 1           | 4  |
| 23  | d1    | 74/74 (100%)   | 53 (72%)  | 21 (28%) | 0           | 1  |
| 24  | D2    | 110/110 (100%) | 89 (81%)  | 21 (19%) | 1           | 5  |
| 24  | d2    | 110/110 (100%) | 95 (86%)  | 15 (14%) | 3           | 13 |
| 25  | D3    | 119/119 (100%) | 94 (79%)  | 25 (21%) | 1           | 4  |
| 25  | d3    | 119/119 (100%) | 98 (82%)  | 21 (18%) | 2           | 7  |
| 26  | D4    | 112/112 (100%) | 91 (81%)  | 21 (19%) | 1           | 5  |
| 26  | d4    | 112/112 (100%) | 91 (81%)  | 21 (19%) | 1           | 5  |
| 27  | D5    | 61/88 (69%)    | 43 (70%)  | 18 (30%) | 0           | 1  |
| 27  | d5    | 61/88 (69%)    | 53 (87%)  | 8 (13%)  | 4           | 14 |
| 28  | D6    | 83/83 (100%)   | 60 (72%)  | 23 (28%) | 0           | 1  |
| 28  | d6    | 83/83 (100%)   | 72 (87%)  | 11 (13%) | 4           | 14 |
| 29  | D7    | 70/70 (100%)   | 57 (81%)  | 13 (19%) | 1           | 5  |
| 29  | d7    | 70/70 (100%)   | 59 (84%)  | 11 (16%) | 2           | 9  |
| 30  | D8    | 56/59 (95%)    | 41 (73%)  | 15 (27%) | 0           | 1  |
| 30  | d8    | 56/59 (95%)    | 46 (82%)  | 10 (18%) | 2           | 6  |
| 31  | D9    | 47/48 (98%)    | 40 (85%)  | 7 (15%)  | 3           | 10 |
| 31  | d9    | 47/48 (98%)    | 37 (79%)  | 10 (21%) | 1           | 4  |
| 32  | E0    | 51/51 (100%)   | 41 (80%)  | 10 (20%) | 1           | 5  |
| 33  | E1    | 62/66 (94%)    | 47 (76%)  | 15 (24%) | 1           | 2  |
| 33  | e1    | 66/66 (100%)   | 47 (71%)  | 19 (29%) | 0           | 1  |
| 34  | SR    | 260/261 (100%) | 234 (90%) | 26 (10%) | 7           | 24 |
| 34  | sR    | 260/261 (100%) | 234 (90%) | 26 (10%) | 7           | 24 |
| 35  | SM    | 97/228 (42%)   | 77 (79%)  | 20 (21%) | 1           | 4  |
| 35  | sM    | 54/228 (24%)   | 46 (85%)  | 8 (15%)  | 3           | 10 |
| 39  | L2    | 193/195 (99%)  | 153 (79%) | 40 (21%) | 1           | 4  |
| 39  | l2    | 192/195 (98%)  | 146 (76%) | 46 (24%) | 1           | 2  |
| 40  | L3    | 321/322 (100%) | 249 (78%) | 72 (22%) | 1           | 3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 40  | l3    | 320/322 (99%)  | 246 (77%) | 74 (23%) | 1           | 3  |
| 41  | L4    | 288/288 (100%) | 229 (80%) | 59 (20%) | 1           | 4  |
| 41  | l4    | 288/288 (100%) | 228 (79%) | 60 (21%) | 1           | 4  |
| 42  | L5    | 244/244 (100%) | 194 (80%) | 50 (20%) | 1           | 4  |
| 42  | l5    | 243/244 (100%) | 183 (75%) | 60 (25%) | 1           | 2  |
| 43  | L6    | 134/152 (88%)  | 112 (84%) | 22 (16%) | 2           | 8  |
| 43  | l6    | 135/152 (89%)  | 108 (80%) | 27 (20%) | 1           | 4  |
| 44  | L7    | 186/204 (91%)  | 159 (86%) | 27 (14%) | 3           | 11 |
| 44  | l7    | 187/204 (92%)  | 160 (86%) | 27 (14%) | 3           | 11 |
| 45  | L8    | 187/207 (90%)  | 154 (82%) | 33 (18%) | 2           | 7  |
| 45  | l8    | 177/207 (86%)  | 143 (81%) | 34 (19%) | 1           | 5  |
| 46  | L9    | 171/171 (100%) | 139 (81%) | 32 (19%) | 1           | 5  |
| 46  | l9    | 171/171 (100%) | 135 (79%) | 36 (21%) | 1           | 4  |
| 47  | M0    | 177/186 (95%)  | 142 (80%) | 35 (20%) | 1           | 5  |
| 47  | m0    | 179/186 (96%)  | 136 (76%) | 43 (24%) | 1           | 2  |
| 48  | M1    | 147/150 (98%)  | 118 (80%) | 29 (20%) | 1           | 5  |
| 48  | m1    | 147/150 (98%)  | 117 (80%) | 30 (20%) | 1           | 4  |
| 49  | M3    | 154/158 (98%)  | 126 (82%) | 28 (18%) | 2           | 6  |
| 49  | m3    | 154/158 (98%)  | 129 (84%) | 25 (16%) | 2           | 8  |
| 50  | M4    | 107/108 (99%)  | 85 (79%)  | 22 (21%) | 1           | 4  |
| 50  | m4    | 108/108 (100%) | 85 (79%)  | 23 (21%) | 1           | 4  |
| 51  | M5    | 175/175 (100%) | 144 (82%) | 31 (18%) | 2           | 6  |
| 51  | m5    | 175/175 (100%) | 146 (83%) | 29 (17%) | 2           | 8  |
| 52  | M6    | 160/161 (99%)  | 130 (81%) | 30 (19%) | 1           | 5  |
| 52  | m6    | 160/161 (99%)  | 125 (78%) | 35 (22%) | 1           | 3  |
| 53  | M7    | 140/145 (97%)  | 105 (75%) | 35 (25%) | 0           | 2  |
| 53  | m7    | 125/145 (86%)  | 104 (83%) | 21 (17%) | 2           | 8  |
| 54  | M8    | 150/150 (100%) | 118 (79%) | 32 (21%) | 1           | 4  |
| 54  | m8    | 150/150 (100%) | 119 (79%) | 31 (21%) | 1           | 4  |
| 55  | M9    | 153/153 (100%) | 129 (84%) | 24 (16%) | 2           | 9  |
| 55  | m9    | 153/153 (100%) | 119 (78%) | 34 (22%) | 1           | 3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 56  | N0    | 156/156 (100%) | 124 (80%) | 32 (20%) | 1           | 4  |
| 56  | n0    | 156/156 (100%) | 124 (80%) | 32 (20%) | 1           | 4  |
| 57  | N1    | 136/136 (100%) | 105 (77%) | 31 (23%) | 1           | 3  |
| 57  | n1    | 136/136 (100%) | 110 (81%) | 26 (19%) | 1           | 5  |
| 58  | N2    | 87/106 (82%)   | 74 (85%)  | 13 (15%) | 3           | 10 |
| 58  | n2    | 85/106 (80%)   | 70 (82%)  | 15 (18%) | 2           | 7  |
| 59  | N3    | 104/104 (100%) | 87 (84%)  | 17 (16%) | 2           | 8  |
| 59  | n3    | 104/104 (100%) | 95 (91%)  | 9 (9%)   | 9           | 30 |
| 60  | N4    | 57/129 (44%)   | 51 (90%)  | 6 (10%)  | 6           | 22 |
| 60  | n4    | 100/129 (78%)  | 85 (85%)  | 15 (15%) | 3           | 10 |
| 61  | N5    | 104/117 (89%)  | 78 (75%)  | 26 (25%) | 0           | 2  |
| 61  | n5    | 104/117 (89%)  | 77 (74%)  | 27 (26%) | 0           | 2  |
| 62  | N6    | 109/109 (100%) | 84 (77%)  | 25 (23%) | 1           | 3  |
| 62  | n6    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 1           | 3  |
| 63  | N7    | 115/115 (100%) | 89 (77%)  | 26 (23%) | 1           | 3  |
| 63  | n7    | 115/115 (100%) | 88 (76%)  | 27 (24%) | 1           | 3  |
| 64  | N8    | 118/118 (100%) | 95 (80%)  | 23 (20%) | 1           | 5  |
| 64  | n8    | 118/118 (100%) | 93 (79%)  | 25 (21%) | 1           | 4  |
| 65  | N9    | 46/46 (100%)   | 37 (80%)  | 9 (20%)  | 1           | 5  |
| 65  | n9    | 46/46 (100%)   | 34 (74%)  | 12 (26%) | 0           | 2  |
| 66  | O0    | 81/87 (93%)    | 65 (80%)  | 16 (20%) | 1           | 5  |
| 66  | o0    | 84/87 (97%)    | 68 (81%)  | 16 (19%) | 1           | 5  |
| 67  | O1    | 92/96 (96%)    | 70 (76%)  | 22 (24%) | 1           | 3  |
| 67  | o1    | 94/96 (98%)    | 71 (76%)  | 23 (24%) | 1           | 2  |
| 68  | O2    | 109/110 (99%)  | 91 (84%)  | 18 (16%) | 2           | 8  |
| 68  | o2    | 109/110 (99%)  | 90 (83%)  | 19 (17%) | 2           | 7  |
| 69  | O3    | 90/90 (100%)   | 76 (84%)  | 14 (16%) | 2           | 9  |
| 69  | o3    | 90/90 (100%)   | 82 (91%)  | 8 (9%)   | 9           | 29 |
| 70  | O4    | 95/101 (94%)   | 74 (78%)  | 21 (22%) | 1           | 3  |
| 70  | o4    | 95/101 (94%)   | 78 (82%)  | 17 (18%) | 2           | 6  |
| 71  | O5    | 104/104 (100%) | 82 (79%)  | 22 (21%) | 1           | 4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 71  | o5    | 103/104 (99%)     | 75 (73%)    | 28 (27%)   | 0           | 1  |
| 72  | O6    | 81/81 (100%)      | 58 (72%)    | 23 (28%)   | 0           | 1  |
| 72  | o6    | 80/81 (99%)       | 53 (66%)    | 27 (34%)   | 0           | 0  |
| 73  | O7    | 70/70 (100%)      | 55 (79%)    | 15 (21%)   | 1           | 4  |
| 73  | o7    | 70/70 (100%)      | 59 (84%)    | 11 (16%)   | 2           | 9  |
| 74  | O8    | 68/68 (100%)      | 54 (79%)    | 14 (21%)   | 1           | 4  |
| 74  | o8    | 67/68 (98%)       | 57 (85%)    | 10 (15%)   | 3           | 10 |
| 75  | O9    | 45/45 (100%)      | 35 (78%)    | 10 (22%)   | 1           | 3  |
| 75  | o9    | 45/45 (100%)      | 32 (71%)    | 13 (29%)   | 0           | 1  |
| 76  | Q0    | 47/47 (100%)      | 38 (81%)    | 9 (19%)    | 1           | 5  |
| 76  | q0    | 47/47 (100%)      | 38 (81%)    | 9 (19%)    | 1           | 5  |
| 77  | Q1    | 23/23 (100%)      | 15 (65%)    | 8 (35%)    | 0           | 0  |
| 77  | q1    | 23/23 (100%)      | 13 (56%)    | 10 (44%)   | 0           | 0  |
| 78  | Q2    | 90/90 (100%)      | 71 (79%)    | 19 (21%)   | 1           | 4  |
| 78  | q2    | 90/90 (100%)      | 71 (79%)    | 19 (21%)   | 1           | 4  |
| 79  | Q3    | 71/71 (100%)      | 55 (78%)    | 16 (22%)   | 1           | 3  |
| 79  | q3    | 71/71 (100%)      | 57 (80%)    | 14 (20%)   | 1           | 5  |
| 80  | e0    | 53/53 (100%)      | 40 (76%)    | 13 (24%)   | 1           | 2  |
| 82  | p0    | 105/253 (42%)     | 81 (77%)    | 24 (23%)   | 1           | 3  |
| All | All   | 18729/20239 (92%) | 14953 (80%) | 3776 (20%) | 1           | 4  |

All (3776) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S0    | 24  | LEU  |
| 2   | S0    | 27  | ARG  |
| 2   | S0    | 34  | GLU  |
| 2   | S0    | 37  | VAL  |
| 2   | S0    | 43  | ASP  |
| 2   | S0    | 50  | VAL  |
| 2   | S0    | 52  | LYS  |
| 2   | S0    | 62  | ARG  |
| 2   | S0    | 80  | THR  |
| 2   | S0    | 84  | ARG  |
| 2   | S0    | 87  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S0    | 88  | LYS  |
| 2   | S0    | 93  | THR  |
| 2   | S0    | 96  | THR  |
| 2   | S0    | 101 | ARG  |
| 2   | S0    | 111 | ILE  |
| 2   | S0    | 131 | GLN  |
| 2   | S0    | 133 | ILE  |
| 2   | S0    | 135 | GLU  |
| 2   | S0    | 153 | SER  |
| 2   | S0    | 154 | GLU  |
| 2   | S0    | 156 | VAL  |
| 2   | S0    | 157 | ASP  |
| 2   | S0    | 169 | SER  |
| 2   | S0    | 170 | ILE  |
| 2   | S0    | 172 | LEU  |
| 2   | S0    | 177 | LEU  |
| 2   | S0    | 181 | VAL  |
| 2   | S0    | 184 | LEU  |
| 2   | S0    | 185 | ARG  |
| 2   | S0    | 188 | LEU  |
| 2   | S0    | 196 | SER  |
| 2   | S0    | 197 | ILE  |
| 3   | S1    | 21  | VAL  |
| 3   | S1    | 25  | THR  |
| 3   | S1    | 29  | TRP  |
| 3   | S1    | 30  | PHE  |
| 3   | S1    | 46  | THR  |
| 3   | S1    | 61  | LEU  |
| 3   | S1    | 65  | VAL  |
| 3   | S1    | 70  | LEU  |
| 3   | S1    | 74  | GLN  |
| 3   | S1    | 79  | HIS  |
| 3   | S1    | 81  | PHE  |
| 3   | S1    | 89  | ASP  |
| 3   | S1    | 97  | LEU  |
| 3   | S1    | 98  | THR  |
| 3   | S1    | 105 | PHE  |
| 3   | S1    | 110 | LEU  |
| 3   | S1    | 135 | LEU  |
| 3   | S1    | 137 | ILE  |
| 3   | S1    | 154 | SER  |
| 3   | S1    | 169 | SER  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | S1    | 170 | GLU  |
| 3   | S1    | 174 | LYS  |
| 3   | S1    | 176 | VAL  |
| 3   | S1    | 180 | THR  |
| 3   | S1    | 181 | LEU  |
| 3   | S1    | 198 | GLU  |
| 3   | S1    | 214 | LYS  |
| 3   | S1    | 215 | VAL  |
| 3   | S1    | 218 | LEU  |
| 3   | S1    | 220 | GLN  |
| 4   | S2    | 41  | LEU  |
| 4   | S2    | 53  | ILE  |
| 4   | S2    | 55  | GLU  |
| 4   | S2    | 58  | LEU  |
| 4   | S2    | 64  | LYS  |
| 4   | S2    | 68  | ILE  |
| 4   | S2    | 69  | ILE  |
| 4   | S2    | 71  | THR  |
| 4   | S2    | 72  | LEU  |
| 4   | S2    | 76  | LEU  |
| 4   | S2    | 77  | GLN  |
| 4   | S2    | 80  | VAL  |
| 4   | S2    | 89  | GLN  |
| 4   | S2    | 90  | THR  |
| 4   | S2    | 91  | ARG  |
| 4   | S2    | 95  | ARG  |
| 4   | S2    | 96  | THR  |
| 4   | S2    | 97  | ARG  |
| 4   | S2    | 103 | VAL  |
| 4   | S2    | 111 | VAL  |
| 4   | S2    | 117 | THR  |
| 4   | S2    | 121 | VAL  |
| 4   | S2    | 130 | ILE  |
| 4   | S2    | 134 | LEU  |
| 4   | S2    | 137 | ILE  |
| 4   | S2    | 139 | ILE  |
| 4   | S2    | 140 | ARG  |
| 4   | S2    | 141 | ARG  |
| 4   | S2    | 146 | THR  |
| 4   | S2    | 148 | LEU  |
| 4   | S2    | 166 | THR  |
| 4   | S2    | 181 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | S2    | 185 | LYS  |
| 4   | S2    | 195 | ASP  |
| 4   | S2    | 206 | THR  |
| 4   | S2    | 207 | LEU  |
| 4   | S2    | 208 | GLU  |
| 4   | S2    | 218 | ILE  |
| 4   | S2    | 222 | TYR  |
| 4   | S2    | 225 | LEU  |
| 4   | S2    | 226 | THR  |
| 4   | S2    | 235 | LEU  |
| 4   | S2    | 237 | VAL  |
| 4   | S2    | 242 | ILE  |
| 4   | S2    | 245 | ASP  |
| 4   | S2    | 246 | GLU  |
| 5   | S3    | 4   | LEU  |
| 5   | S3    | 5   | ILE  |
| 5   | S3    | 10  | LYS  |
| 5   | S3    | 12  | VAL  |
| 5   | S3    | 23  | GLU  |
| 5   | S3    | 39  | VAL  |
| 5   | S3    | 41  | VAL  |
| 5   | S3    | 56  | GLN  |
| 5   | S3    | 65  | ARG  |
| 5   | S3    | 67  | ASN  |
| 5   | S3    | 81  | PRO  |
| 5   | S3    | 84  | ILE  |
| 5   | S3    | 89  | GLU  |
| 5   | S3    | 92  | GLN  |
| 5   | S3    | 93  | ASP  |
| 5   | S3    | 105 | MET  |
| 5   | S3    | 111 | ASN  |
| 5   | S3    | 117 | ARG  |
| 5   | S3    | 127 | MET  |
| 5   | S3    | 134 | CYS  |
| 5   | S3    | 142 | LEU  |
| 5   | S3    | 151 | LYS  |
| 5   | S3    | 158 | ILE  |
| 5   | S3    | 172 | THR  |
| 5   | S3    | 175 | VAL  |
| 5   | S3    | 176 | LEU  |
| 5   | S3    | 178 | ARG  |
| 5   | S3    | 181 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | S3    | 182 | LEU  |
| 5   | S3    | 187 | LYS  |
| 5   | S3    | 202 | LEU  |
| 5   | S3    | 204 | ASP  |
| 5   | S3    | 209 | ILE  |
| 5   | S3    | 217 | ILE  |
| 5   | S3    | 220 | PRO  |
| 5   | S3    | 222 | VAL  |
| 5   | S3    | 223 | LYS  |
| 6   | S4    | 6   | LYS  |
| 6   | S4    | 7   | LYS  |
| 6   | S4    | 9   | LEU  |
| 6   | S4    | 12  | LEU  |
| 6   | S4    | 23  | LEU  |
| 6   | S4    | 37  | LYS  |
| 6   | S4    | 38  | LEU  |
| 6   | S4    | 45  | ILE  |
| 6   | S4    | 48  | LEU  |
| 6   | S4    | 62  | LYS  |
| 6   | S4    | 65  | LEU  |
| 6   | S4    | 67  | GLN  |
| 6   | S4    | 68  | ARG  |
| 6   | S4    | 70  | VAL  |
| 6   | S4    | 72  | VAL  |
| 6   | S4    | 77  | ARG  |
| 6   | S4    | 89  | VAL  |
| 6   | S4    | 92  | LEU  |
| 6   | S4    | 95  | THR  |
| 6   | S4    | 102 | VAL  |
| 6   | S4    | 105 | VAL  |
| 6   | S4    | 115 | THR  |
| 6   | S4    | 116 | ASP  |
| 6   | S4    | 123 | LEU  |
| 6   | S4    | 126 | VAL  |
| 6   | S4    | 131 | LEU  |
| 6   | S4    | 133 | LYS  |
| 6   | S4    | 155 | LYS  |
| 6   | S4    | 158 | ASP  |
| 6   | S4    | 160 | VAL  |
| 6   | S4    | 180 | LEU  |
| 6   | S4    | 181 | VAL  |
| 6   | S4    | 187 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | S4    | 197 | HIS  |
| 6   | S4    | 198 | LYS  |
| 6   | S4    | 211 | LYS  |
| 6   | S4    | 214 | LEU  |
| 6   | S4    | 215 | ASP  |
| 6   | S4    | 221 | ARG  |
| 6   | S4    | 222 | LEU  |
| 6   | S4    | 227 | VAL  |
| 6   | S4    | 236 | ILE  |
| 6   | S4    | 240 | LYS  |
| 6   | S4    | 242 | LYS  |
| 6   | S4    | 248 | ILE  |
| 6   | S4    | 258 | GLN  |
| 7   | S5    | 23  | VAL  |
| 7   | S5    | 25  | LEU  |
| 7   | S5    | 38  | THR  |
| 7   | S5    | 41  | LYS  |
| 7   | S5    | 43  | PHE  |
| 7   | S5    | 45  | LYS  |
| 7   | S5    | 53  | VAL  |
| 7   | S5    | 76  | ARG  |
| 7   | S5    | 79  | ASN  |
| 7   | S5    | 84  | LYS  |
| 7   | S5    | 89  | ILE  |
| 7   | S5    | 93  | LEU  |
| 7   | S5    | 94  | THR  |
| 7   | S5    | 99  | MET  |
| 7   | S5    | 109 | LYS  |
| 7   | S5    | 119 | ASP  |
| 7   | S5    | 139 | ASN  |
| 7   | S5    | 146 | THR  |
| 7   | S5    | 147 | THR  |
| 7   | S5    | 148 | ARG  |
| 7   | S5    | 149 | VAL  |
| 7   | S5    | 156 | ARG  |
| 7   | S5    | 160 | VAL  |
| 7   | S5    | 162 | VAL  |
| 7   | S5    | 185 | ARG  |
| 7   | S5    | 190 | ILE  |
| 7   | S5    | 193 | THR  |
| 7   | S5    | 194 | LEU  |
| 7   | S5    | 225 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | S6    | 9   | VAL  |
| 8   | S6    | 13  | GLN  |
| 8   | S6    | 21  | GLU  |
| 8   | S6    | 25  | ARG  |
| 8   | S6    | 30  | LYS  |
| 8   | S6    | 44  | GLU  |
| 8   | S6    | 65  | GLN  |
| 8   | S6    | 67  | VAL  |
| 8   | S6    | 76  | LEU  |
| 8   | S6    | 78  | THR  |
| 8   | S6    | 79  | LYS  |
| 8   | S6    | 80  | ASN  |
| 8   | S6    | 82  | SER  |
| 8   | S6    | 87  | ARG  |
| 8   | S6    | 97  | VAL  |
| 8   | S6    | 98  | ARG  |
| 8   | S6    | 120 | GLU  |
| 8   | S6    | 124 | LEU  |
| 8   | S6    | 126 | ASP  |
| 8   | S6    | 127 | THR  |
| 8   | S6    | 128 | THR  |
| 8   | S6    | 129 | VAL  |
| 8   | S6    | 132 | ARG  |
| 8   | S6    | 133 | LEU  |
| 8   | S6    | 137 | ARG  |
| 8   | S6    | 142 | ARG  |
| 8   | S6    | 143 | LYS  |
| 8   | S6    | 150 | GLU  |
| 8   | S6    | 155 | ASP  |
| 8   | S6    | 158 | ILE  |
| 8   | S6    | 169 | TYR  |
| 8   | S6    | 174 | LYS  |
| 8   | S6    | 175 | ILE  |
| 8   | S6    | 176 | GLN  |
| 8   | S6    | 177 | ARG  |
| 8   | S6    | 179 | VAL  |
| 8   | S6    | 211 | LEU  |
| 8   | S6    | 212 | LEU  |
| 8   | S6    | 223 | LYS  |
| 9   | S7    | 8   | ILE  |
| 9   | S7    | 14  | THR  |
| 9   | S7    | 15  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | S7    | 25  | VAL  |
| 9   | S7    | 37  | GLU  |
| 9   | S7    | 38  | LEU  |
| 9   | S7    | 46  | ILE  |
| 9   | S7    | 49  | ILE  |
| 9   | S7    | 50  | ASP  |
| 9   | S7    | 51  | VAL  |
| 9   | S7    | 60  | ILE  |
| 9   | S7    | 67  | LEU  |
| 9   | S7    | 70  | PHE  |
| 9   | S7    | 73  | VAL  |
| 9   | S7    | 75  | THR  |
| 9   | S7    | 77  | LEU  |
| 9   | S7    | 87  | ASP  |
| 9   | S7    | 95  | GLU  |
| 9   | S7    | 97  | ARG  |
| 9   | S7    | 104 | ARG  |
| 9   | S7    | 105 | THR  |
| 9   | S7    | 109 | VAL  |
| 9   | S7    | 111 | LYS  |
| 9   | S7    | 114 | ARG  |
| 9   | S7    | 116 | ARG  |
| 9   | S7    | 126 | LEU  |
| 9   | S7    | 130 | VAL  |
| 9   | S7    | 136 | VAL  |
| 9   | S7    | 143 | LEU  |
| 9   | S7    | 144 | VAL  |
| 9   | S7    | 167 | GLU  |
| 9   | S7    | 184 | GLU  |
| 9   | S7    | 185 | ILE  |
| 10  | S8    | 17  | LYS  |
| 10  | S8    | 20  | GLN  |
| 10  | S8    | 25  | ARG  |
| 10  | S8    | 28  | GLU  |
| 10  | S8    | 29  | LEU  |
| 10  | S8    | 32  | GLN  |
| 10  | S8    | 36  | THR  |
| 10  | S8    | 43  | ILE  |
| 10  | S8    | 46  | VAL  |
| 10  | S8    | 58  | LEU  |
| 10  | S8    | 60  | ILE  |
| 10  | S8    | 72  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | S8    | 73  | SER  |
| 10  | S8    | 82  | VAL  |
| 10  | S8    | 135 | LYS  |
| 10  | S8    | 138 | ASN  |
| 10  | S8    | 151 | LYS  |
| 10  | S8    | 152 | ILE  |
| 10  | S8    | 155 | SER  |
| 10  | S8    | 164 | ARG  |
| 10  | S8    | 184 | LEU  |
| 10  | S8    | 185 | GLU  |
| 10  | S8    | 196 | LEU  |
| 11  | S9    | 3   | ARG  |
| 11  | S9    | 6   | ARG  |
| 11  | S9    | 7   | THR  |
| 11  | S9    | 10  | LYS  |
| 11  | S9    | 14  | THR  |
| 11  | S9    | 22  | SER  |
| 11  | S9    | 28  | LEU  |
| 11  | S9    | 39  | LYS  |
| 11  | S9    | 49  | LEU  |
| 11  | S9    | 60  | LEU  |
| 11  | S9    | 78  | ARG  |
| 11  | S9    | 82  | ARG  |
| 11  | S9    | 89  | ASP  |
| 11  | S9    | 92  | LYS  |
| 11  | S9    | 93  | LEU  |
| 11  | S9    | 96  | VAL  |
| 11  | S9    | 97  | LEU  |
| 11  | S9    | 99  | LEU  |
| 11  | S9    | 100 | LYS  |
| 11  | S9    | 101 | VAL  |
| 11  | S9    | 105 | LEU  |
| 11  | S9    | 109 | LEU  |
| 11  | S9    | 110 | GLN  |
| 11  | S9    | 111 | THR  |
| 11  | S9    | 113 | VAL  |
| 11  | S9    | 122 | VAL  |
| 11  | S9    | 133 | HIS  |
| 11  | S9    | 134 | ILE  |
| 11  | S9    | 138 | LYS  |
| 11  | S9    | 143 | ILE  |
| 11  | S9    | 149 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | S9    | 151 | ASP  |
| 11  | S9    | 156 | ILE  |
| 11  | S9    | 161 | THR  |
| 11  | S9    | 171 | ARG  |
| 11  | S9    | 172 | VAL  |
| 11  | S9    | 182 | GLU  |
| 12  | C0    | 5   | LYS  |
| 12  | C0    | 11  | ILE  |
| 12  | C0    | 20  | VAL  |
| 12  | C0    | 22  | VAL  |
| 12  | C0    | 24  | LYS  |
| 12  | C0    | 29  | GLN  |
| 12  | C0    | 31  | LYS  |
| 12  | C0    | 32  | HIS  |
| 12  | C0    | 40  | LEU  |
| 12  | C0    | 46  | LEU  |
| 12  | C0    | 50  | THR  |
| 12  | C0    | 55  | VAL  |
| 12  | C0    | 67  | THR  |
| 12  | C0    | 71  | GLU  |
| 12  | C0    | 76  | LEU  |
| 12  | C0    | 78  | GLU  |
| 12  | C0    | 81  | ASN  |
| 12  | C0    | 82  | LEU  |
| 13  | C1    | 7   | VAL  |
| 13  | C1    | 8   | GLN  |
| 13  | C1    | 21  | ASN  |
| 13  | C1    | 27  | THR  |
| 13  | C1    | 29  | LYS  |
| 13  | C1    | 37  | ASN  |
| 13  | C1    | 40  | LEU  |
| 13  | C1    | 43  | LYS  |
| 13  | C1    | 44  | THR  |
| 13  | C1    | 54  | ILE  |
| 13  | C1    | 56  | LYS  |
| 13  | C1    | 66  | ILE  |
| 13  | C1    | 67  | ARG  |
| 13  | C1    | 74  | THR  |
| 13  | C1    | 76  | VAL  |
| 13  | C1    | 79  | LYS  |
| 13  | C1    | 83  | THR  |
| 13  | C1    | 94  | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | C1    | 99  | ARG  |
| 13  | C1    | 109 | VAL  |
| 13  | C1    | 117 | VAL  |
| 13  | C1    | 118 | GLN  |
| 13  | C1    | 123 | VAL  |
| 13  | C1    | 131 | ILE  |
| 13  | C1    | 140 | VAL  |
| 13  | C1    | 141 | LYS  |
| 13  | C1    | 143 | SER  |
| 14  | C2    | 28  | LEU  |
| 14  | C2    | 33  | ARG  |
| 14  | C2    | 43  | ARG  |
| 14  | C2    | 46  | ARG  |
| 14  | C2    | 50  | LYS  |
| 14  | C2    | 52  | LEU  |
| 14  | C2    | 54  | ARG  |
| 14  | C2    | 59  | LEU  |
| 14  | C2    | 61  | VAL  |
| 14  | C2    | 66  | VAL  |
| 14  | C2    | 71  | ILE  |
| 14  | C2    | 73  | LYS  |
| 14  | C2    | 74  | LEU  |
| 14  | C2    | 86  | VAL  |
| 14  | C2    | 89  | ILE  |
| 14  | C2    | 97  | LEU  |
| 14  | C2    | 103 | LEU  |
| 14  | C2    | 129 | GLU  |
| 14  | C2    | 132 | GLU  |
| 14  | C2    | 135 | MET  |
| 14  | C2    | 139 | HIS  |
| 14  | C2    | 140 | PHE  |
| 15  | C3    | 3   | ARG  |
| 15  | C3    | 9   | LYS  |
| 15  | C3    | 11  | ILE  |
| 15  | C3    | 16  | ILE  |
| 15  | C3    | 27  | LYS  |
| 15  | C3    | 32  | SER  |
| 15  | C3    | 33  | VAL  |
| 15  | C3    | 39  | LYS  |
| 15  | C3    | 45  | LEU  |
| 15  | C3    | 56  | ASP  |
| 15  | C3    | 64  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | C3    | 66  | ILE  |
| 15  | C3    | 74  | ILE  |
| 15  | C3    | 77  | SER  |
| 15  | C3    | 83  | GLU  |
| 15  | C3    | 84  | ILE  |
| 15  | C3    | 88  | LEU  |
| 15  | C3    | 102 | LEU  |
| 15  | C3    | 114 | ARG  |
| 15  | C3    | 115 | LEU  |
| 15  | C3    | 125 | LEU  |
| 15  | C3    | 127 | ARG  |
| 15  | C3    | 134 | VAL  |
| 15  | C3    | 143 | SER  |
| 15  | C3    | 145 | THR  |
| 15  | C3    | 149 | LEU  |
| 15  | C3    | 150 | VAL  |
| 16  | C4    | 13  | VAL  |
| 16  | C4    | 16  | VAL  |
| 16  | C4    | 24  | ASN  |
| 16  | C4    | 29  | HIS  |
| 16  | C4    | 30  | VAL  |
| 16  | C4    | 31  | THR  |
| 16  | C4    | 39  | ILE  |
| 16  | C4    | 42  | VAL  |
| 16  | C4    | 51  | ASP  |
| 16  | C4    | 55  | SER  |
| 16  | C4    | 56  | SER  |
| 16  | C4    | 81  | VAL  |
| 16  | C4    | 92  | LYS  |
| 16  | C4    | 102 | LEU  |
| 16  | C4    | 103 | ARG  |
| 16  | C4    | 107 | ARG  |
| 16  | C4    | 123 | SER  |
| 16  | C4    | 132 | ARG  |
| 16  | C4    | 136 | ARG  |
| 16  | C4    | 137 | LEU  |
| 17  | C5    | 11  | VAL  |
| 17  | C5    | 13  | LYS  |
| 17  | C5    | 20  | VAL  |
| 17  | C5    | 21  | ASP  |
| 17  | C5    | 22  | LEU  |
| 17  | C5    | 28  | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | C5    | 31  | GLU  |
| 17  | C5    | 34  | VAL  |
| 17  | C5    | 35  | LYS  |
| 17  | C5    | 36  | LEU  |
| 17  | C5    | 44  | ARG  |
| 17  | C5    | 47  | ARG  |
| 17  | C5    | 52  | LYS  |
| 17  | C5    | 84  | ILE  |
| 17  | C5    | 92  | SER  |
| 17  | C5    | 110 | GLU  |
| 17  | C5    | 124 | THR  |
| 18  | C6    | 12  | LYS  |
| 18  | C6    | 14  | LYS  |
| 18  | C6    | 17  | THR  |
| 18  | C6    | 26  | LYS  |
| 18  | C6    | 29  | ILE  |
| 18  | C6    | 39  | VAL  |
| 18  | C6    | 44  | LEU  |
| 18  | C6    | 45  | ARG  |
| 18  | C6    | 53  | LEU  |
| 18  | C6    | 54  | LEU  |
| 18  | C6    | 57  | LEU  |
| 18  | C6    | 66  | ARG  |
| 18  | C6    | 69  | VAL  |
| 18  | C6    | 98  | ASP  |
| 18  | C6    | 101 | SER  |
| 18  | C6    | 106 | LYS  |
| 18  | C6    | 114 | ARG  |
| 18  | C6    | 116 | LEU  |
| 18  | C6    | 118 | ILE  |
| 18  | C6    | 123 | ARG  |
| 18  | C6    | 128 | LYS  |
| 18  | C6    | 137 | ARG  |
| 18  | C6    | 143 | ARG  |
| 19  | C7    | 7   | LYS  |
| 19  | C7    | 8   | THR  |
| 19  | C7    | 26  | LEU  |
| 19  | C7    | 29  | GLN  |
| 19  | C7    | 30  | THR  |
| 19  | C7    | 34  | LEU  |
| 19  | C7    | 38  | ILE  |
| 19  | C7    | 46  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | C7    | 49  | LYS  |
| 19  | C7    | 54  | THR  |
| 19  | C7    | 61  | ILE  |
| 19  | C7    | 62  | GLN  |
| 19  | C7    | 69  | ILE  |
| 19  | C7    | 72  | LYS  |
| 19  | C7    | 78  | ARG  |
| 19  | C7    | 83  | GLN  |
| 19  | C7    | 88  | VAL  |
| 19  | C7    | 105 | GLN  |
| 19  | C7    | 107 | SER  |
| 19  | C7    | 113 | LEU  |
| 19  | C7    | 115 | LEU  |
| 19  | C7    | 119 | LEU  |
| 20  | C8    | 3   | LEU  |
| 20  | C8    | 5   | VAL  |
| 20  | C8    | 6   | GLN  |
| 20  | C8    | 8   | GLN  |
| 20  | C8    | 11  | PHE  |
| 20  | C8    | 13  | HIS  |
| 20  | C8    | 14  | ILE  |
| 20  | C8    | 18  | LEU  |
| 20  | C8    | 20  | THR  |
| 20  | C8    | 25  | ASN  |
| 20  | C8    | 26  | ILE  |
| 20  | C8    | 28  | ILE  |
| 20  | C8    | 40  | ARG  |
| 20  | C8    | 46  | VAL  |
| 20  | C8    | 57  | ARG  |
| 20  | C8    | 60  | GLU  |
| 20  | C8    | 61  | LEU  |
| 20  | C8    | 71  | GLN  |
| 20  | C8    | 77  | THR  |
| 20  | C8    | 80  | LYS  |
| 20  | C8    | 92  | ILE  |
| 20  | C8    | 105 | VAL  |
| 20  | C8    | 107 | SER  |
| 20  | C8    | 110 | ARG  |
| 20  | C8    | 116 | LEU  |
| 20  | C8    | 119 | ILE  |
| 20  | C8    | 132 | ARG  |
| 20  | C8    | 136 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | C8    | 143 | ARG  |
| 21  | C9    | 4   | VAL  |
| 21  | C9    | 6   | VAL  |
| 21  | C9    | 22  | LEU  |
| 21  | C9    | 28  | LEU  |
| 21  | C9    | 33  | TYR  |
| 21  | C9    | 34  | VAL  |
| 21  | C9    | 35  | ASP  |
| 21  | C9    | 36  | ILE  |
| 21  | C9    | 37  | VAL  |
| 21  | C9    | 38  | LYS  |
| 21  | C9    | 53  | TRP  |
| 21  | C9    | 57  | ARG  |
| 21  | C9    | 67  | MET  |
| 21  | C9    | 68  | ARG  |
| 21  | C9    | 84  | LYS  |
| 21  | C9    | 86  | ARG  |
| 21  | C9    | 88  | VAL  |
| 21  | C9    | 94  | ILE  |
| 21  | C9    | 100 | ILE  |
| 21  | C9    | 111 | ILE  |
| 21  | C9    | 131 | ASP  |
| 21  | C9    | 132 | LEU  |
| 21  | C9    | 144 | GLU  |
| 22  | D0    | 15  | GLN  |
| 22  | D0    | 17  | GLN  |
| 22  | D0    | 18  | GLN  |
| 22  | D0    | 20  | ILE  |
| 22  | D0    | 22  | ILE  |
| 22  | D0    | 23  | ARG  |
| 22  | D0    | 25  | THR  |
| 22  | D0    | 27  | THR  |
| 22  | D0    | 30  | LYS  |
| 22  | D0    | 34  | LEU  |
| 22  | D0    | 43  | LYS  |
| 22  | D0    | 46  | GLU  |
| 22  | D0    | 47  | GLN  |
| 22  | D0    | 51  | VAL  |
| 22  | D0    | 57  | ARG  |
| 22  | D0    | 60  | THR  |
| 22  | D0    | 64  | LYS  |
| 22  | D0    | 66  | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | D0    | 67  | THR  |
| 22  | D0    | 72  | ASN  |
| 22  | D0    | 74  | GLU  |
| 22  | D0    | 76  | SER  |
| 22  | D0    | 81  | THR  |
| 22  | D0    | 88  | LYS  |
| 22  | D0    | 89  | ARG  |
| 22  | D0    | 97  | VAL  |
| 22  | D0    | 99  | ILE  |
| 22  | D0    | 103 | ILE  |
| 22  | D0    | 108 | ILE  |
| 22  | D0    | 114 | VAL  |
| 22  | D0    | 117 | VAL  |
| 22  | D0    | 121 | ASN  |
| 23  | D1    | 1   | MET  |
| 23  | D1    | 7   | GLN  |
| 23  | D1    | 8   | LEU  |
| 23  | D1    | 9   | VAL  |
| 23  | D1    | 11  | LEU  |
| 23  | D1    | 16  | LYS  |
| 23  | D1    | 25  | LYS  |
| 23  | D1    | 32  | VAL  |
| 23  | D1    | 34  | ILE  |
| 23  | D1    | 39  | VAL  |
| 23  | D1    | 41  | GLU  |
| 23  | D1    | 52  | THR  |
| 23  | D1    | 62  | ARG  |
| 23  | D1    | 69  | LEU  |
| 23  | D1    | 78  | LEU  |
| 24  | D2    | 4   | SER  |
| 24  | D2    | 6   | VAL  |
| 24  | D2    | 7   | LEU  |
| 24  | D2    | 12  | ASN  |
| 24  | D2    | 22  | LYS  |
| 24  | D2    | 23  | ARG  |
| 24  | D2    | 24  | GLN  |
| 24  | D2    | 25  | VAL  |
| 24  | D2    | 29  | PRO  |
| 24  | D2    | 49  | GLU  |
| 24  | D2    | 53  | ILE  |
| 24  | D2    | 65  | LEU  |
| 24  | D2    | 86  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | D2    | 93  | LEU  |
| 24  | D2    | 98  | GLN  |
| 24  | D2    | 103 | ILE  |
| 24  | D2    | 105 | THR  |
| 24  | D2    | 110 | ILE  |
| 24  | D2    | 121 | VAL  |
| 24  | D2    | 125 | ILE  |
| 24  | D2    | 129 | VAL  |
| 25  | D3    | 7   | ARG  |
| 25  | D3    | 9   | LEU  |
| 25  | D3    | 14  | LYS  |
| 25  | D3    | 26  | GLU  |
| 25  | D3    | 28  | ASN  |
| 25  | D3    | 33  | LEU  |
| 25  | D3    | 60  | GLU  |
| 25  | D3    | 69  | ARG  |
| 25  | D3    | 73  | ARG  |
| 25  | D3    | 77  | ILE  |
| 25  | D3    | 82  | LYS  |
| 25  | D3    | 83  | VAL  |
| 25  | D3    | 84  | THR  |
| 25  | D3    | 101 | GLU  |
| 25  | D3    | 103 | LEU  |
| 25  | D3    | 107 | PHE  |
| 25  | D3    | 109 | ARG  |
| 25  | D3    | 110 | LYS  |
| 25  | D3    | 114 | LYS  |
| 25  | D3    | 117 | ILE  |
| 25  | D3    | 131 | SER  |
| 25  | D3    | 132 | LEU  |
| 25  | D3    | 133 | LEU  |
| 25  | D3    | 139 | LYS  |
| 25  | D3    | 144 | ARG  |
| 26  | D4    | 2   | SER  |
| 26  | D4    | 10  | ARG  |
| 26  | D4    | 17  | LEU  |
| 26  | D4    | 32  | ARG  |
| 26  | D4    | 34  | ASN  |
| 26  | D4    | 36  | SER  |
| 26  | D4    | 46  | GLU  |
| 26  | D4    | 51  | GLU  |
| 26  | D4    | 57  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | D4    | 61  | ARG  |
| 26  | D4    | 62  | THR  |
| 26  | D4    | 75  | VAL  |
| 26  | D4    | 81  | GLU  |
| 26  | D4    | 84  | LYS  |
| 26  | D4    | 88  | THR  |
| 26  | D4    | 99  | LYS  |
| 26  | D4    | 102 | LYS  |
| 26  | D4    | 121 | THR  |
| 26  | D4    | 124 | ARG  |
| 26  | D4    | 128 | LYS  |
| 26  | D4    | 133 | ASN  |
| 27  | D5    | 40  | VAL  |
| 27  | D5    | 42  | LEU  |
| 27  | D5    | 49  | ARG  |
| 27  | D5    | 50  | ILE  |
| 27  | D5    | 58  | ARG  |
| 27  | D5    | 60  | VAL  |
| 27  | D5    | 63  | SER  |
| 27  | D5    | 69  | LEU  |
| 27  | D5    | 71  | ILE  |
| 27  | D5    | 75  | LEU  |
| 27  | D5    | 78  | ILE  |
| 27  | D5    | 85  | LYS  |
| 27  | D5    | 92  | ILE  |
| 27  | D5    | 95  | HIS  |
| 27  | D5    | 97  | LYS  |
| 27  | D5    | 98  | GLN  |
| 27  | D5    | 100 | ILE  |
| 27  | D5    | 102 | THR  |
| 28  | D6    | 4   | LYS  |
| 28  | D6    | 10  | ARG  |
| 28  | D6    | 12  | LYS  |
| 28  | D6    | 15  | ARG  |
| 28  | D6    | 30  | ILE  |
| 28  | D6    | 36  | ILE  |
| 28  | D6    | 41  | ILE  |
| 28  | D6    | 44  | ILE  |
| 28  | D6    | 45  | VAL  |
| 28  | D6    | 46  | GLU  |
| 28  | D6    | 50  | VAL  |
| 28  | D6    | 58  | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | D6    | 61  | GLU  |
| 28  | D6    | 64  | LEU  |
| 28  | D6    | 67  | THR  |
| 28  | D6    | 68  | TYR  |
| 28  | D6    | 69  | ASN  |
| 28  | D6    | 71  | LEU  |
| 28  | D6    | 83  | ILE  |
| 28  | D6    | 84  | VAL  |
| 28  | D6    | 85  | ARG  |
| 28  | D6    | 87  | ARG  |
| 28  | D6    | 90  | GLU  |
| 29  | D7    | 2   | VAL  |
| 29  | D7    | 3   | LEU  |
| 29  | D7    | 4   | VAL  |
| 29  | D7    | 20  | LYS  |
| 29  | D7    | 29  | ARG  |
| 29  | D7    | 33  | LEU  |
| 29  | D7    | 42  | ASN  |
| 29  | D7    | 43  | ILE  |
| 29  | D7    | 55  | THR  |
| 29  | D7    | 60  | SER  |
| 29  | D7    | 62  | ILE  |
| 29  | D7    | 67  | THR  |
| 29  | D7    | 73  | LEU  |
| 30  | D8    | 9   | LEU  |
| 30  | D8    | 13  | ILE  |
| 30  | D8    | 14  | LYS  |
| 30  | D8    | 15  | VAL  |
| 30  | D8    | 19  | THR  |
| 30  | D8    | 28  | VAL  |
| 30  | D8    | 35  | ASP  |
| 30  | D8    | 36  | THR  |
| 30  | D8    | 39  | THR  |
| 30  | D8    | 44  | VAL  |
| 30  | D8    | 48  | VAL  |
| 30  | D8    | 49  | ARG  |
| 30  | D8    | 52  | ASP  |
| 30  | D8    | 59  | SER  |
| 30  | D8    | 64  | ARG  |
| 31  | D9    | 6   | VAL  |
| 31  | D9    | 12  | ARG  |
| 31  | D9    | 19  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | D9    | 22  | ARG  |
| 31  | D9    | 28  | THR  |
| 31  | D9    | 30  | LEU  |
| 31  | D9    | 39  | CYS  |
| 32  | E0    | 3   | LYS  |
| 32  | E0    | 21  | VAL  |
| 32  | E0    | 25  | GLU  |
| 32  | E0    | 28  | LYS  |
| 32  | E0    | 39  | LEU  |
| 32  | E0    | 42  | ARG  |
| 32  | E0    | 43  | ARG  |
| 32  | E0    | 47  | VAL  |
| 32  | E0    | 49  | LEU  |
| 32  | E0    | 53  | LYS  |
| 33  | E1    | 84  | VAL  |
| 33  | E1    | 86  | THR  |
| 33  | E1    | 89  | LYS  |
| 33  | E1    | 91  | ILE  |
| 33  | E1    | 93  | HIS  |
| 33  | E1    | 97  | LYS  |
| 33  | E1    | 102 | VAL  |
| 33  | E1    | 108 | VAL  |
| 33  | E1    | 113 | LYS  |
| 33  | E1    | 119 | ARG  |
| 33  | E1    | 120 | GLU  |
| 33  | E1    | 130 | VAL  |
| 33  | E1    | 146 | SER  |
| 33  | E1    | 147 | VAL  |
| 33  | E1    | 150 | VAL  |
| 34  | SR    | 6   | VAL  |
| 34  | SR    | 7   | LEU  |
| 34  | SR    | 10  | ARG  |
| 34  | SR    | 29  | GLN  |
| 34  | SR    | 76  | ASP  |
| 34  | SR    | 96  | THR  |
| 34  | SR    | 117 | LYS  |
| 34  | SR    | 123 | ILE  |
| 34  | SR    | 129 | LYS  |
| 34  | SR    | 136 | ILE  |
| 34  | SR    | 137 | LYS  |
| 34  | SR    | 152 | SER  |
| 34  | SR    | 165 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | SR    | 166 | SER  |
| 34  | SR    | 188 | ILE  |
| 34  | SR    | 191 | ASP  |
| 34  | SR    | 195 | HIS  |
| 34  | SR    | 196 | ASN  |
| 34  | SR    | 199 | ILE  |
| 34  | SR    | 211 | ILE  |
| 34  | SR    | 229 | LYS  |
| 34  | SR    | 238 | ASP  |
| 34  | SR    | 265 | LEU  |
| 34  | SR    | 300 | THR  |
| 34  | SR    | 316 | MET  |
| 34  | SR    | 317 | THR  |
| 35  | SM    | 25  | ILE  |
| 35  | SM    | 33  | LYS  |
| 35  | SM    | 34  | LYS  |
| 35  | SM    | 49  | LYS  |
| 35  | SM    | 51  | ARG  |
| 35  | SM    | 53  | ARG  |
| 35  | SM    | 61  | ILE  |
| 35  | SM    | 64  | LYS  |
| 35  | SM    | 68  | ARG  |
| 35  | SM    | 79  | SER  |
| 35  | SM    | 84  | LYS  |
| 35  | SM    | 89  | ARG  |
| 35  | SM    | 91  | THR  |
| 35  | SM    | 97  | THR  |
| 35  | SM    | 100 | THR  |
| 35  | SM    | 102 | THR  |
| 35  | SM    | 103 | LYS  |
| 35  | SM    | 116 | GLU  |
| 35  | SM    | 131 | ILE  |
| 35  | SM    | 139 | GLU  |
| 39  | L2    | 10  | LYS  |
| 39  | L2    | 20  | THR  |
| 39  | L2    | 23  | ARG  |
| 39  | L2    | 32  | LEU  |
| 39  | L2    | 36  | GLU  |
| 39  | L2    | 44  | ILE  |
| 39  | L2    | 45  | VAL  |
| 39  | L2    | 48  | ILE  |
| 39  | L2    | 49  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | L2    | 62  | VAL  |
| 39  | L2    | 70  | ARG  |
| 39  | L2    | 74  | GLU  |
| 39  | L2    | 82  | VAL  |
| 39  | L2    | 88  | ILE  |
| 39  | L2    | 96  | LEU  |
| 39  | L2    | 101 | VAL  |
| 39  | L2    | 104 | LEU  |
| 39  | L2    | 112 | ILE  |
| 39  | L2    | 116 | VAL  |
| 39  | L2    | 134 | VAL  |
| 39  | L2    | 137 | ILE  |
| 39  | L2    | 141 | PRO  |
| 39  | L2    | 142 | ASP  |
| 39  | L2    | 143 | GLU  |
| 39  | L2    | 146 | THR  |
| 39  | L2    | 157 | VAL  |
| 39  | L2    | 158 | ILE  |
| 39  | L2    | 165 | VAL  |
| 39  | L2    | 169 | ILE  |
| 39  | L2    | 177 | LYS  |
| 39  | L2    | 179 | LEU  |
| 39  | L2    | 181 | LYS  |
| 39  | L2    | 190 | ARG  |
| 39  | L2    | 191 | LEU  |
| 39  | L2    | 202 | VAL  |
| 39  | L2    | 204 | MET  |
| 39  | L2    | 207 | VAL  |
| 39  | L2    | 225 | ILE  |
| 39  | L2    | 227 | ARG  |
| 39  | L2    | 230 | VAL  |
| 40  | L3    | 3   | HIS  |
| 40  | L3    | 7   | GLU  |
| 40  | L3    | 10  | ARG  |
| 40  | L3    | 17  | LEU  |
| 40  | L3    | 19  | ARG  |
| 40  | L3    | 25  | ILE  |
| 40  | L3    | 37  | ARG  |
| 40  | L3    | 39  | LYS  |
| 40  | L3    | 43  | LEU  |
| 40  | L3    | 47  | LEU  |
| 40  | L3    | 56  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | L3    | 70  | ARG  |
| 40  | L3    | 73  | VAL  |
| 40  | L3    | 79  | VAL  |
| 40  | L3    | 84  | VAL  |
| 40  | L3    | 85  | VAL  |
| 40  | L3    | 103 | THR  |
| 40  | L3    | 110 | LEU  |
| 40  | L3    | 111 | SER  |
| 40  | L3    | 114 | VAL  |
| 40  | L3    | 116 | ARG  |
| 40  | L3    | 121 | ASN  |
| 40  | L3    | 124 | LYS  |
| 40  | L3    | 134 | SER  |
| 40  | L3    | 139 | GLN  |
| 40  | L3    | 146 | ARG  |
| 40  | L3    | 148 | LEU  |
| 40  | L3    | 150 | ARG  |
| 40  | L3    | 156 | SER  |
| 40  | L3    | 157 | VAL  |
| 40  | L3    | 162 | VAL  |
| 40  | L3    | 169 | THR  |
| 40  | L3    | 173 | GLN  |
| 40  | L3    | 175 | LYS  |
| 40  | L3    | 183 | LEU  |
| 40  | L3    | 188 | ILE  |
| 40  | L3    | 192 | VAL  |
| 40  | L3    | 196 | ARG  |
| 40  | L3    | 200 | GLU  |
| 40  | L3    | 202 | THR  |
| 40  | L3    | 205 | VAL  |
| 40  | L3    | 210 | GLU  |
| 40  | L3    | 221 | THR  |
| 40  | L3    | 229 | VAL  |
| 40  | L3    | 232 | ARG  |
| 40  | L3    | 235 | THR  |
| 40  | L3    | 236 | LYS  |
| 40  | L3    | 238 | LEU  |
| 40  | L3    | 242 | THR  |
| 40  | L3    | 244 | ARG  |
| 40  | L3    | 252 | ILE  |
| 40  | L3    | 264 | VAL  |
| 40  | L3    | 275 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | L3    | 281 | LYS  |
| 40  | L3    | 284 | ARG  |
| 40  | L3    | 296 | THR  |
| 40  | L3    | 305 | ILE  |
| 40  | L3    | 320 | ASP  |
| 40  | L3    | 324 | VAL  |
| 40  | L3    | 328 | ILE  |
| 40  | L3    | 331 | ASN  |
| 40  | L3    | 332 | ARG  |
| 40  | L3    | 338 | LEU  |
| 40  | L3    | 344 | THR  |
| 40  | L3    | 346 | THR  |
| 40  | L3    | 347 | SER  |
| 40  | L3    | 349 | LYS  |
| 40  | L3    | 352 | GLU  |
| 40  | L3    | 355 | SER  |
| 40  | L3    | 361 | THR  |
| 40  | L3    | 364 | LYS  |
| 40  | L3    | 380 | MET  |
| 41  | L4    | 4   | PRO  |
| 41  | L4    | 22  | LEU  |
| 41  | L4    | 25  | VAL  |
| 41  | L4    | 40  | THR  |
| 41  | L4    | 52  | VAL  |
| 41  | L4    | 53  | SER  |
| 41  | L4    | 60  | THR  |
| 41  | L4    | 69  | ARG  |
| 41  | L4    | 71  | VAL  |
| 41  | L4    | 74  | ILE  |
| 41  | L4    | 85  | SER  |
| 41  | L4    | 93  | MET  |
| 41  | L4    | 112 | LYS  |
| 41  | L4    | 117 | GLU  |
| 41  | L4    | 122 | THR  |
| 41  | L4    | 136 | LEU  |
| 41  | L4    | 138 | ARG  |
| 41  | L4    | 144 | LYS  |
| 41  | L4    | 148 | ILE  |
| 41  | L4    | 150 | LEU  |
| 41  | L4    | 152 | VAL  |
| 41  | L4    | 156 | LEU  |
| 41  | L4    | 161 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | L4    | 170 | LYS  |
| 41  | L4    | 172 | VAL  |
| 41  | L4    | 176 | SER  |
| 41  | L4    | 177 | ASP  |
| 41  | L4    | 179 | LEU  |
| 41  | L4    | 182 | LEU  |
| 41  | L4    | 185 | LYS  |
| 41  | L4    | 188 | ARG  |
| 41  | L4    | 193 | LYS  |
| 41  | L4    | 200 | THR  |
| 41  | L4    | 203 | ARG  |
| 41  | L4    | 206 | LEU  |
| 41  | L4    | 216 | VAL  |
| 41  | L4    | 220 | ARG  |
| 41  | L4    | 222 | VAL  |
| 41  | L4    | 226 | GLU  |
| 41  | L4    | 230 | VAL  |
| 41  | L4    | 233 | LEU  |
| 41  | L4    | 246 | ARG  |
| 41  | L4    | 258 | LEU  |
| 41  | L4    | 267 | VAL  |
| 41  | L4    | 283 | THR  |
| 41  | L4    | 306 | THR  |
| 41  | L4    | 307 | GLN  |
| 41  | L4    | 311 | HIS  |
| 41  | L4    | 313 | LEU  |
| 41  | L4    | 323 | VAL  |
| 41  | L4    | 327 | LEU  |
| 41  | L4    | 333 | VAL  |
| 41  | L4    | 339 | LEU  |
| 41  | L4    | 346 | LYS  |
| 41  | L4    | 349 | THR  |
| 41  | L4    | 350 | LYS  |
| 41  | L4    | 354 | VAL  |
| 41  | L4    | 358 | THR  |
| 41  | L4    | 359 | LEU  |
| 42  | L5    | 5   | LYS  |
| 42  | L5    | 10  | SER  |
| 42  | L5    | 23  | ARG  |
| 42  | L5    | 35  | ARG  |
| 42  | L5    | 41  | LYS  |
| 42  | L5    | 64  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | L5    | 65  | ILE  |
| 42  | L5    | 68  | THR  |
| 42  | L5    | 69  | ILE  |
| 42  | L5    | 75  | LEU  |
| 42  | L5    | 92  | LEU  |
| 42  | L5    | 101 | THR  |
| 42  | L5    | 105 | ILE  |
| 42  | L5    | 109 | THR  |
| 42  | L5    | 110 | LEU  |
| 42  | L5    | 112 | LYS  |
| 42  | L5    | 113 | LEU  |
| 42  | L5    | 115 | LEU  |
| 42  | L5    | 118 | THR  |
| 42  | L5    | 122 | VAL  |
| 42  | L5    | 128 | GLU  |
| 42  | L5    | 131 | LEU  |
| 42  | L5    | 140 | ARG  |
| 42  | L5    | 144 | VAL  |
| 42  | L5    | 146 | LEU  |
| 42  | L5    | 148 | ILE  |
| 42  | L5    | 151 | GLN  |
| 42  | L5    | 152 | ARG  |
| 42  | L5    | 155 | THR  |
| 42  | L5    | 163 | LEU  |
| 42  | L5    | 177 | GLU  |
| 42  | L5    | 194 | LEU  |
| 42  | L5    | 196 | ARG  |
| 42  | L5    | 205 | SER  |
| 42  | L5    | 216 | GLU  |
| 42  | L5    | 217 | GLU  |
| 42  | L5    | 222 | LEU  |
| 42  | L5    | 232 | ASP  |
| 42  | L5    | 234 | ASP  |
| 42  | L5    | 236 | LEU  |
| 42  | L5    | 239 | ILE  |
| 42  | L5    | 254 | LYS  |
| 42  | L5    | 257 | GLU  |
| 42  | L5    | 261 | THR  |
| 42  | L5    | 263 | GLU  |
| 42  | L5    | 273 | ARG  |
| 42  | L5    | 275 | THR  |
| 42  | L5    | 279 | LYS  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | L5    | 290 | ILE  |
| 42  | L5    | 293 | LEU  |
| 43  | L6    | 2   | SER  |
| 43  | L6    | 5   | LYS  |
| 43  | L6    | 8   | LYS  |
| 43  | L6    | 12  | SER  |
| 43  | L6    | 21  | THR  |
| 43  | L6    | 31  | ARG  |
| 43  | L6    | 52  | VAL  |
| 43  | L6    | 59  | GLU  |
| 43  | L6    | 64  | LEU  |
| 43  | L6    | 65  | ILE  |
| 43  | L6    | 78  | ARG  |
| 43  | L6    | 79  | VAL  |
| 43  | L6    | 84  | VAL  |
| 43  | L6    | 89  | THR  |
| 43  | L6    | 90  | LYS  |
| 43  | L6    | 93  | VAL  |
| 43  | L6    | 94  | GLU  |
| 43  | L6    | 98  | VAL  |
| 43  | L6    | 129 | GLU  |
| 43  | L6    | 134 | ARG  |
| 43  | L6    | 152 | THR  |
| 43  | L6    | 155 | LEU  |
| 44  | L7    | 24  | GLU  |
| 44  | L7    | 25  | GLN  |
| 44  | L7    | 26  | VAL  |
| 44  | L7    | 38  | LYS  |
| 44  | L7    | 45  | LEU  |
| 44  | L7    | 54  | GLU  |
| 44  | L7    | 77  | VAL  |
| 44  | L7    | 82  | LYS  |
| 44  | L7    | 83  | LEU  |
| 44  | L7    | 88  | ARG  |
| 44  | L7    | 89  | ILE  |
| 44  | L7    | 92  | ILE  |
| 44  | L7    | 95  | ILE  |
| 44  | L7    | 98  | LYS  |
| 44  | L7    | 100 | ARG  |
| 44  | L7    | 110 | ARG  |
| 44  | L7    | 121 | LYS  |
| 44  | L7    | 124 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | L7    | 143 | THR  |
| 44  | L7    | 157 | ASN  |
| 44  | L7    | 158 | LYS  |
| 44  | L7    | 164 | SER  |
| 44  | L7    | 175 | LYS  |
| 44  | L7    | 179 | LEU  |
| 44  | L7    | 184 | LEU  |
| 44  | L7    | 239 | LEU  |
| 44  | L7    | 244 | ASN  |
| 45  | L8    | 26  | LEU  |
| 45  | L8    | 27  | THR  |
| 45  | L8    | 41  | GLN  |
| 45  | L8    | 47  | SER  |
| 45  | L8    | 50  | VAL  |
| 45  | L8    | 61  | GLN  |
| 45  | L8    | 63  | LYS  |
| 45  | L8    | 71  | VAL  |
| 45  | L8    | 74  | THR  |
| 45  | L8    | 79  | GLN  |
| 45  | L8    | 81  | THR  |
| 45  | L8    | 84  | ARG  |
| 45  | L8    | 95  | ASN  |
| 45  | L8    | 110 | THR  |
| 45  | L8    | 118 | GLU  |
| 45  | L8    | 132 | VAL  |
| 45  | L8    | 136 | LEU  |
| 45  | L8    | 149 | LYS  |
| 45  | L8    | 150 | LEU  |
| 45  | L8    | 156 | ASP  |
| 45  | L8    | 160 | ILE  |
| 45  | L8    | 163 | VAL  |
| 45  | L8    | 169 | LEU  |
| 45  | L8    | 172 | LYS  |
| 45  | L8    | 180 | VAL  |
| 45  | L8    | 185 | ARG  |
| 45  | L8    | 189 | LEU  |
| 45  | L8    | 203 | VAL  |
| 45  | L8    | 204 | ARG  |
| 45  | L8    | 214 | LEU  |
| 45  | L8    | 238 | LEU  |
| 45  | L8    | 246 | MET  |
| 45  | L8    | 251 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | L9    | 4   | ILE  |
| 46  | L9    | 5   | GLN  |
| 46  | L9    | 9   | GLN  |
| 46  | L9    | 14  | GLU  |
| 46  | L9    | 16  | VAL  |
| 46  | L9    | 18  | VAL  |
| 46  | L9    | 22  | SER  |
| 46  | L9    | 33  | THR  |
| 46  | L9    | 41  | ILE  |
| 46  | L9    | 48  | VAL  |
| 46  | L9    | 52  | LEU  |
| 46  | L9    | 62  | ARG  |
| 46  | L9    | 68  | LEU  |
| 46  | L9    | 69  | ARG  |
| 46  | L9    | 70  | THR  |
| 46  | L9    | 80  | THR  |
| 46  | L9    | 82  | VAL  |
| 46  | L9    | 121 | LYS  |
| 46  | L9    | 124 | ARG  |
| 46  | L9    | 132 | VAL  |
| 46  | L9    | 135 | GLU  |
| 46  | L9    | 137 | SER  |
| 46  | L9    | 138 | THR  |
| 46  | L9    | 139 | ASN  |
| 46  | L9    | 150 | SER  |
| 46  | L9    | 151 | VAL  |
| 46  | L9    | 161 | LEU  |
| 46  | L9    | 162 | GLN  |
| 46  | L9    | 166 | ARG  |
| 46  | L9    | 173 | ARG  |
| 46  | L9    | 188 | THR  |
| 46  | L9    | 189 | GLU  |
| 47  | M0    | 18  | PRO  |
| 47  | M0    | 24  | ARG  |
| 47  | M0    | 26  | VAL  |
| 47  | M0    | 31  | ILE  |
| 47  | M0    | 32  | ARG  |
| 47  | M0    | 33  | ILE  |
| 47  | M0    | 36  | LEU  |
| 47  | M0    | 40  | LYS  |
| 47  | M0    | 42  | THR  |
| 47  | M0    | 48  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | M0    | 52  | LEU  |
| 47  | M0    | 57  | LEU  |
| 47  | M0    | 63  | GLU  |
| 47  | M0    | 69  | ARG  |
| 47  | M0    | 74  | LYS  |
| 47  | M0    | 76  | MET  |
| 47  | M0    | 77  | THR  |
| 47  | M0    | 78  | THR  |
| 47  | M0    | 87  | LEU  |
| 47  | M0    | 91  | VAL  |
| 47  | M0    | 99  | ILE  |
| 47  | M0    | 129 | VAL  |
| 47  | M0    | 130 | ASP  |
| 47  | M0    | 138 | VAL  |
| 47  | M0    | 140 | THR  |
| 47  | M0    | 143 | SER  |
| 47  | M0    | 163 | GLN  |
| 47  | M0    | 165 | ILE  |
| 47  | M0    | 166 | ILE  |
| 47  | M0    | 169 | LYS  |
| 47  | M0    | 174 | THR  |
| 47  | M0    | 178 | ARG  |
| 47  | M0    | 185 | ARG  |
| 47  | M0    | 197 | VAL  |
| 47  | M0    | 203 | LYS  |
| 48  | M1    | 6   | GLN  |
| 48  | M1    | 9   | MET  |
| 48  | M1    | 10  | ARG  |
| 48  | M1    | 12  | LEU  |
| 48  | M1    | 13  | LYS  |
| 48  | M1    | 16  | LYS  |
| 48  | M1    | 17  | LEU  |
| 48  | M1    | 23  | VAL  |
| 48  | M1    | 30  | LEU  |
| 48  | M1    | 31  | THR  |
| 48  | M1    | 40  | LEU  |
| 48  | M1    | 44  | THR  |
| 48  | M1    | 46  | VAL  |
| 48  | M1    | 65  | ILE  |
| 48  | M1    | 70  | THR  |
| 48  | M1    | 80  | LEU  |
| 48  | M1    | 88  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | M1    | 94  | ARG  |
| 48  | M1    | 106 | ILE  |
| 48  | M1    | 107 | ASP  |
| 48  | M1    | 112 | LEU  |
| 48  | M1    | 115 | LYS  |
| 48  | M1    | 120 | ILE  |
| 48  | M1    | 130 | VAL  |
| 48  | M1    | 138 | VAL  |
| 48  | M1    | 140 | ARG  |
| 48  | M1    | 142 | LYS  |
| 48  | M1    | 161 | SER  |
| 48  | M1    | 166 | LYS  |
| 49  | M3    | 23  | LYS  |
| 49  | M3    | 34  | SER  |
| 49  | M3    | 45  | LYS  |
| 49  | M3    | 46  | ILE  |
| 49  | M3    | 54  | LEU  |
| 49  | M3    | 55  | ARG  |
| 49  | M3    | 57  | VAL  |
| 49  | M3    | 58  | VAL  |
| 49  | M3    | 59  | ARG  |
| 49  | M3    | 63  | VAL  |
| 49  | M3    | 67  | ARG  |
| 49  | M3    | 69  | VAL  |
| 49  | M3    | 85  | LEU  |
| 49  | M3    | 93  | ILE  |
| 49  | M3    | 107 | GLU  |
| 49  | M3    | 114 | GLN  |
| 49  | M3    | 117 | LYS  |
| 49  | M3    | 122 | LYS  |
| 49  | M3    | 124 | ILE  |
| 49  | M3    | 128 | ARG  |
| 49  | M3    | 131 | LYS  |
| 49  | M3    | 144 | THR  |
| 49  | M3    | 164 | GLU  |
| 49  | M3    | 165 | SER  |
| 49  | M3    | 171 | ARG  |
| 49  | M3    | 182 | ILE  |
| 49  | M3    | 190 | LYS  |
| 49  | M3    | 194 | GLU  |
| 50  | M4    | 8   | LYS  |
| 50  | M4    | 15  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | M4    | 20  | VAL  |
| 50  | M4    | 27  | GLN  |
| 50  | M4    | 43  | LYS  |
| 50  | M4    | 50  | LYS  |
| 50  | M4    | 53  | VAL  |
| 50  | M4    | 59  | ASN  |
| 50  | M4    | 63  | VAL  |
| 50  | M4    | 64  | VAL  |
| 50  | M4    | 66  | THR  |
| 50  | M4    | 72  | LEU  |
| 50  | M4    | 90  | VAL  |
| 50  | M4    | 91  | CYS  |
| 50  | M4    | 92  | GLU  |
| 50  | M4    | 102 | LYS  |
| 50  | M4    | 105 | GLN  |
| 50  | M4    | 108 | ARG  |
| 50  | M4    | 113 | THR  |
| 50  | M4    | 125 | LYS  |
| 50  | M4    | 126 | GLN  |
| 50  | M4    | 130 | THR  |
| 51  | M5    | 10  | LEU  |
| 51  | M5    | 15  | GLN  |
| 51  | M5    | 20  | ARG  |
| 51  | M5    | 22  | LEU  |
| 51  | M5    | 38  | ARG  |
| 51  | M5    | 49  | ARG  |
| 51  | M5    | 50  | ARG  |
| 51  | M5    | 68  | ARG  |
| 51  | M5    | 75  | VAL  |
| 51  | M5    | 80  | THR  |
| 51  | M5    | 83  | LYS  |
| 51  | M5    | 85  | THR  |
| 51  | M5    | 92  | LEU  |
| 51  | M5    | 96  | ARG  |
| 51  | M5    | 97  | SER  |
| 51  | M5    | 98  | LEU  |
| 51  | M5    | 105 | ARG  |
| 51  | M5    | 106 | VAL  |
| 51  | M5    | 109 | ARG  |
| 51  | M5    | 113 | LEU  |
| 51  | M5    | 133 | ILE  |
| 51  | M5    | 151 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | M5    | 155 | VAL  |
| 51  | M5    | 170 | LYS  |
| 51  | M5    | 182 | ASN  |
| 51  | M5    | 183 | THR  |
| 51  | M5    | 187 | ARG  |
| 51  | M5    | 188 | ARG  |
| 51  | M5    | 190 | THR  |
| 51  | M5    | 194 | GLN  |
| 51  | M5    | 204 | LYS  |
| 52  | M6    | 22  | VAL  |
| 52  | M6    | 25  | LYS  |
| 52  | M6    | 33  | ILE  |
| 52  | M6    | 34  | VAL  |
| 52  | M6    | 41  | LEU  |
| 52  | M6    | 46  | GLU  |
| 52  | M6    | 66  | LYS  |
| 52  | M6    | 67  | THR  |
| 52  | M6    | 78  | ARG  |
| 52  | M6    | 79  | ILE  |
| 52  | M6    | 82  | LYS  |
| 52  | M6    | 84  | LEU  |
| 52  | M6    | 85  | ARG  |
| 52  | M6    | 106 | GLU  |
| 52  | M6    | 110 | PRO  |
| 52  | M6    | 116 | LYS  |
| 52  | M6    | 117 | ARG  |
| 52  | M6    | 124 | LEU  |
| 52  | M6    | 126 | VAL  |
| 52  | M6    | 128 | ARG  |
| 52  | M6    | 134 | LYS  |
| 52  | M6    | 143 | THR  |
| 52  | M6    | 160 | ARG  |
| 52  | M6    | 161 | LYS  |
| 52  | M6    | 166 | GLU  |
| 52  | M6    | 170 | LYS  |
| 52  | M6    | 175 | THR  |
| 52  | M6    | 180 | SER  |
| 52  | M6    | 189 | ASP  |
| 52  | M6    | 190 | VAL  |
| 53  | M7    | 9   | THR  |
| 53  | M7    | 24  | VAL  |
| 53  | M7    | 29  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | M7    | 32  | THR  |
| 53  | M7    | 36  | ILE  |
| 53  | M7    | 52  | LEU  |
| 53  | M7    | 53  | ASP  |
| 53  | M7    | 56  | ARG  |
| 53  | M7    | 65  | SER  |
| 53  | M7    | 67  | ILE  |
| 53  | M7    | 69  | ARG  |
| 53  | M7    | 74  | LYS  |
| 53  | M7    | 78  | VAL  |
| 53  | M7    | 89  | LYS  |
| 53  | M7    | 91  | VAL  |
| 53  | M7    | 94  | LEU  |
| 53  | M7    | 107 | LEU  |
| 53  | M7    | 112 | LEU  |
| 53  | M7    | 114 | VAL  |
| 53  | M7    | 117 | ILE  |
| 53  | M7    | 119 | VAL  |
| 53  | M7    | 124 | LYS  |
| 53  | M7    | 126 | ARG  |
| 53  | M7    | 127 | ARG  |
| 53  | M7    | 128 | ARG  |
| 53  | M7    | 136 | ILE  |
| 53  | M7    | 144 | SER  |
| 53  | M7    | 151 | THR  |
| 53  | M7    | 153 | LYS  |
| 53  | M7    | 157 | VAL  |
| 53  | M7    | 165 | VAL  |
| 53  | M7    | 168 | LEU  |
| 53  | M7    | 169 | THR  |
| 53  | M7    | 180 | LYS  |
| 53  | M7    | 181 | ARG  |
| 54  | M8    | 3   | ILE  |
| 54  | M8    | 17  | THR  |
| 54  | M8    | 24  | VAL  |
| 54  | M8    | 26  | LEU  |
| 54  | M8    | 27  | LYS  |
| 54  | M8    | 31  | LYS  |
| 54  | M8    | 32  | LEU  |
| 54  | M8    | 34  | THR  |
| 54  | M8    | 39  | ARG  |
| 54  | M8    | 41  | ASP  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | M8    | 49  | LEU  |
| 54  | M8    | 50  | LYS  |
| 54  | M8    | 57  | ILE  |
| 54  | M8    | 66  | ARG  |
| 54  | M8    | 69  | ARG  |
| 54  | M8    | 74  | GLU  |
| 54  | M8    | 80  | THR  |
| 54  | M8    | 81  | VAL  |
| 54  | M8    | 86  | THR  |
| 54  | M8    | 93  | ILE  |
| 54  | M8    | 95  | GLU  |
| 54  | M8    | 111 | ARG  |
| 54  | M8    | 122 | ILE  |
| 54  | M8    | 127 | LEU  |
| 54  | M8    | 135 | GLN  |
| 54  | M8    | 138 | LEU  |
| 54  | M8    | 141 | ARG  |
| 54  | M8    | 147 | ARG  |
| 54  | M8    | 150 | VAL  |
| 54  | M8    | 159 | LYS  |
| 54  | M8    | 168 | THR  |
| 54  | M8    | 180 | ARG  |
| 55  | M9    | 10  | LEU  |
| 55  | M9    | 22  | VAL  |
| 55  | M9    | 29  | THR  |
| 55  | M9    | 30  | SER  |
| 55  | M9    | 41  | ILE  |
| 55  | M9    | 44  | LEU  |
| 55  | M9    | 53  | LYS  |
| 55  | M9    | 60  | LYS  |
| 55  | M9    | 74  | ARG  |
| 55  | M9    | 81  | ARG  |
| 55  | M9    | 99  | LEU  |
| 55  | M9    | 100 | ARG  |
| 55  | M9    | 101 | VAL  |
| 55  | M9    | 103 | ARG  |
| 55  | M9    | 104 | ARG  |
| 55  | M9    | 106 | LEU  |
| 55  | M9    | 115 | ILE  |
| 55  | M9    | 116 | ASP  |
| 55  | M9    | 138 | LEU  |
| 55  | M9    | 144 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | M9    | 153 | LYS  |
| 55  | M9    | 160 | GLU  |
| 55  | M9    | 175 | GLN  |
| 55  | M9    | 177 | VAL  |
| 56  | N0    | 1   | MET  |
| 56  | N0    | 8   | GLN  |
| 56  | N0    | 32  | SER  |
| 56  | N0    | 45  | LEU  |
| 56  | N0    | 50  | LYS  |
| 56  | N0    | 51  | VAL  |
| 56  | N0    | 58  | ILE  |
| 56  | N0    | 61  | ILE  |
| 56  | N0    | 64  | ILE  |
| 56  | N0    | 79  | VAL  |
| 56  | N0    | 80  | ARG  |
| 56  | N0    | 87  | THR  |
| 56  | N0    | 97  | VAL  |
| 56  | N0    | 100 | VAL  |
| 56  | N0    | 104 | GLU  |
| 56  | N0    | 105 | THR  |
| 56  | N0    | 115 | ARG  |
| 56  | N0    | 117 | ARG  |
| 56  | N0    | 125 | LYS  |
| 56  | N0    | 130 | GLU  |
| 56  | N0    | 132 | THR  |
| 56  | N0    | 136 | LYS  |
| 56  | N0    | 137 | ARG  |
| 56  | N0    | 138 | GLN  |
| 56  | N0    | 141 | LYS  |
| 56  | N0    | 142 | GLN  |
| 56  | N0    | 145 | THR  |
| 56  | N0    | 155 | ARG  |
| 56  | N0    | 156 | VAL  |
| 56  | N0    | 157 | GLN  |
| 56  | N0    | 167 | ARG  |
| 56  | N0    | 171 | PHE  |
| 57  | N1    | 25  | VAL  |
| 57  | N1    | 26  | HIS  |
| 57  | N1    | 27  | LEU  |
| 57  | N1    | 32  | LYS  |
| 57  | N1    | 43  | LYS  |
| 57  | N1    | 55  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | N1    | 68  | THR  |
| 57  | N1    | 71  | SER  |
| 57  | N1    | 78  | LYS  |
| 57  | N1    | 79  | MET  |
| 57  | N1    | 80  | VAL  |
| 57  | N1    | 83  | ARG  |
| 57  | N1    | 88  | ARG  |
| 57  | N1    | 89  | LEU  |
| 57  | N1    | 96  | ILE  |
| 57  | N1    | 102 | ARG  |
| 57  | N1    | 104 | GLU  |
| 57  | N1    | 106 | LEU  |
| 57  | N1    | 115 | LYS  |
| 57  | N1    | 118 | GLU  |
| 57  | N1    | 124 | VAL  |
| 57  | N1    | 126 | VAL  |
| 57  | N1    | 128 | LEU  |
| 57  | N1    | 139 | ARG  |
| 57  | N1    | 141 | VAL  |
| 57  | N1    | 143 | THR  |
| 57  | N1    | 149 | GLN  |
| 57  | N1    | 154 | VAL  |
| 57  | N1    | 158 | THR  |
| 57  | N1    | 159 | PHE  |
| 57  | N1    | 160 | ILE  |
| 58  | N2    | 10  | LYS  |
| 58  | N2    | 39  | ASP  |
| 58  | N2    | 43  | VAL  |
| 58  | N2    | 44  | GLU  |
| 58  | N2    | 50  | LEU  |
| 58  | N2    | 52  | ASN  |
| 58  | N2    | 54  | VAL  |
| 58  | N2    | 61  | THR  |
| 58  | N2    | 66  | VAL  |
| 58  | N2    | 88  | GLN  |
| 58  | N2    | 93  | ILE  |
| 58  | N2    | 100 | THR  |
| 58  | N2    | 105 | LEU  |
| 59  | N3    | 2   | SER  |
| 59  | N3    | 9   | THR  |
| 59  | N3    | 13  | ILE  |
| 59  | N3    | 32  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | N3    | 48  | ARG  |
| 59  | N3    | 64  | LYS  |
| 59  | N3    | 69  | LEU  |
| 59  | N3    | 72  | LYS  |
| 59  | N3    | 73  | VAL  |
| 59  | N3    | 74  | MET  |
| 59  | N3    | 83  | LYS  |
| 59  | N3    | 91  | VAL  |
| 59  | N3    | 102 | ILE  |
| 59  | N3    | 115 | THR  |
| 59  | N3    | 120 | LYS  |
| 59  | N3    | 133 | SER  |
| 59  | N3    | 137 | VAL  |
| 60  | N4    | 4   | GLU  |
| 60  | N4    | 5   | ILE  |
| 60  | N4    | 26  | SER  |
| 60  | N4    | 39  | LEU  |
| 60  | N4    | 41  | LYS  |
| 60  | N4    | 64  | THR  |
| 61  | N5    | 25  | LYS  |
| 61  | N5    | 27  | ARG  |
| 61  | N5    | 37  | THR  |
| 61  | N5    | 38  | LEU  |
| 61  | N5    | 39  | LYS  |
| 61  | N5    | 40  | LEU  |
| 61  | N5    | 45  | LYS  |
| 61  | N5    | 48  | SER  |
| 61  | N5    | 63  | ILE  |
| 61  | N5    | 71  | THR  |
| 61  | N5    | 73  | MET  |
| 61  | N5    | 75  | LYS  |
| 61  | N5    | 77  | GLU  |
| 61  | N5    | 86  | VAL  |
| 61  | N5    | 104 | GLU  |
| 61  | N5    | 105 | VAL  |
| 61  | N5    | 106 | ASP  |
| 61  | N5    | 108 | LEU  |
| 61  | N5    | 109 | LYS  |
| 61  | N5    | 115 | ARG  |
| 61  | N5    | 125 | ARG  |
| 61  | N5    | 133 | LEU  |
| 61  | N5    | 135 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | N5    | 138 | ARG  |
| 61  | N5    | 139 | ILE  |
| 61  | N5    | 142 | ILE  |
| 62  | N6    | 3   | LYS  |
| 62  | N6    | 5   | SER  |
| 62  | N6    | 8   | VAL  |
| 62  | N6    | 13  | ARG  |
| 62  | N6    | 17  | LYS  |
| 62  | N6    | 26  | GLN  |
| 62  | N6    | 37  | LYS  |
| 62  | N6    | 42  | GLN  |
| 62  | N6    | 45  | ILE  |
| 62  | N6    | 50  | ILE  |
| 62  | N6    | 51  | ARG  |
| 62  | N6    | 55  | GLU  |
| 62  | N6    | 56  | VAL  |
| 62  | N6    | 57  | LEU  |
| 62  | N6    | 70  | ILE  |
| 62  | N6    | 76  | LEU  |
| 62  | N6    | 80  | VAL  |
| 62  | N6    | 88  | GLU  |
| 62  | N6    | 94  | SER  |
| 62  | N6    | 95  | VAL  |
| 62  | N6    | 97  | ILE  |
| 62  | N6    | 105 | VAL  |
| 62  | N6    | 119 | ILE  |
| 62  | N6    | 126 | LEU  |
| 62  | N6    | 127 | GLU  |
| 63  | N7    | 14  | VAL  |
| 63  | N7    | 17  | ARG  |
| 63  | N7    | 24  | VAL  |
| 63  | N7    | 25  | ILE  |
| 63  | N7    | 26  | VAL  |
| 63  | N7    | 30  | ASP  |
| 63  | N7    | 34  | LYS  |
| 63  | N7    | 42  | LEU  |
| 63  | N7    | 46  | ILE  |
| 63  | N7    | 52  | LYS  |
| 63  | N7    | 54  | THR  |
| 63  | N7    | 61  | LYS  |
| 63  | N7    | 64  | LYS  |
| 63  | N7    | 73  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | N7    | 75  | VAL  |
| 63  | N7    | 81  | LEU  |
| 63  | N7    | 83  | THR  |
| 63  | N7    | 86  | THR  |
| 63  | N7    | 87  | LEU  |
| 63  | N7    | 102 | GLU  |
| 63  | N7    | 103 | GLN  |
| 63  | N7    | 108 | GLU  |
| 63  | N7    | 121 | ARG  |
| 63  | N7    | 132 | SER  |
| 63  | N7    | 134 | LEU  |
| 63  | N7    | 135 | ARG  |
| 64  | N8    | 6   | THR  |
| 64  | N8    | 8   | THR  |
| 64  | N8    | 10  | LYS  |
| 64  | N8    | 12  | ARG  |
| 64  | N8    | 16  | SER  |
| 64  | N8    | 29  | PRO  |
| 64  | N8    | 42  | ARG  |
| 64  | N8    | 47  | LYS  |
| 64  | N8    | 58  | MET  |
| 64  | N8    | 65  | GLN  |
| 64  | N8    | 76  | ASP  |
| 64  | N8    | 78  | LEU  |
| 64  | N8    | 84  | GLU  |
| 64  | N8    | 85  | ASP  |
| 64  | N8    | 91  | LEU  |
| 64  | N8    | 92  | LYS  |
| 64  | N8    | 115 | LYS  |
| 64  | N8    | 118 | ILE  |
| 64  | N8    | 120 | ASN  |
| 64  | N8    | 130 | VAL  |
| 64  | N8    | 133 | LEU  |
| 64  | N8    | 138 | ILE  |
| 64  | N8    | 144 | VAL  |
| 65  | N9    | 4   | SER  |
| 65  | N9    | 18  | ARG  |
| 65  | N9    | 22  | LYS  |
| 65  | N9    | 25  | LYS  |
| 65  | N9    | 28  | LYS  |
| 65  | N9    | 33  | LYS  |
| 65  | N9    | 35  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | N9    | 50  | THR  |
| 65  | N9    | 59  | LYS  |
| 66  | O0    | 9   | SER  |
| 66  | O0    | 16  | LEU  |
| 66  | O0    | 18  | ILE  |
| 66  | O0    | 20  | SER  |
| 66  | O0    | 30  | THR  |
| 66  | O0    | 32  | LYS  |
| 66  | O0    | 34  | LEU  |
| 66  | O0    | 48  | THR  |
| 66  | O0    | 61  | MET  |
| 66  | O0    | 66  | LYS  |
| 66  | O0    | 76  | GLU  |
| 66  | O0    | 83  | LYS  |
| 66  | O0    | 87  | VAL  |
| 66  | O0    | 97  | ASP  |
| 66  | O0    | 100 | ILE  |
| 66  | O0    | 101 | LEU  |
| 67  | O1    | 8   | VAL  |
| 67  | O1    | 13  | THR  |
| 67  | O1    | 16  | LEU  |
| 67  | O1    | 28  | ARG  |
| 67  | O1    | 31  | ARG  |
| 67  | O1    | 42  | LEU  |
| 67  | O1    | 46  | THR  |
| 67  | O1    | 47  | ASP  |
| 67  | O1    | 50  | ARG  |
| 67  | O1    | 55  | LEU  |
| 67  | O1    | 64  | VAL  |
| 67  | O1    | 68  | GLU  |
| 67  | O1    | 79  | ARG  |
| 67  | O1    | 81  | GLU  |
| 67  | O1    | 82  | GLU  |
| 67  | O1    | 84  | ASP  |
| 67  | O1    | 89  | LEU  |
| 67  | O1    | 96  | VAL  |
| 67  | O1    | 102 | LYS  |
| 67  | O1    | 106 | THR  |
| 67  | O1    | 107 | VAL  |
| 67  | O1    | 110 | GLU  |
| 68  | O2    | 4   | LEU  |
| 68  | O2    | 8   | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | O2    | 15  | LYS  |
| 68  | O2    | 18  | LYS  |
| 68  | O2    | 19  | ARG  |
| 68  | O2    | 33  | ARG  |
| 68  | O2    | 62  | LYS  |
| 68  | O2    | 73  | THR  |
| 68  | O2    | 75  | LEU  |
| 68  | O2    | 76  | VAL  |
| 68  | O2    | 82  | LEU  |
| 68  | O2    | 87  | MET  |
| 68  | O2    | 91  | THR  |
| 68  | O2    | 105 | ARG  |
| 68  | O2    | 106 | VAL  |
| 68  | O2    | 109 | LEU  |
| 68  | O2    | 125 | ARG  |
| 68  | O2    | 128 | LEU  |
| 69  | O3    | 3   | GLU  |
| 69  | O3    | 10  | LYS  |
| 69  | O3    | 20  | LYS  |
| 69  | O3    | 21  | ARG  |
| 69  | O3    | 48  | ARG  |
| 69  | O3    | 49  | ILE  |
| 69  | O3    | 59  | VAL  |
| 69  | O3    | 60  | ARG  |
| 69  | O3    | 62  | SER  |
| 69  | O3    | 70  | LYS  |
| 69  | O3    | 80  | VAL  |
| 69  | O3    | 81  | VAL  |
| 69  | O3    | 98  | VAL  |
| 69  | O3    | 106 | ASN  |
| 70  | O4    | 5   | VAL  |
| 70  | O4    | 8   | ARG  |
| 70  | O4    | 20  | ILE  |
| 70  | O4    | 23  | VAL  |
| 70  | O4    | 24  | LYS  |
| 70  | O4    | 29  | ILE  |
| 70  | O4    | 31  | ARG  |
| 70  | O4    | 35  | VAL  |
| 70  | O4    | 49  | SER  |
| 70  | O4    | 51  | LEU  |
| 70  | O4    | 56  | THR  |
| 70  | O4    | 58  | ARG  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70  | O4    | 65  | VAL  |
| 70  | O4    | 66  | SER  |
| 70  | O4    | 71  | THR  |
| 70  | O4    | 72  | VAL  |
| 70  | O4    | 81  | CYS  |
| 70  | O4    | 86  | LYS  |
| 70  | O4    | 87  | GLU  |
| 70  | O4    | 90  | ILE  |
| 70  | O4    | 104 | VAL  |
| 71  | O5    | 4   | VAL  |
| 71  | O5    | 21  | LEU  |
| 71  | O5    | 28  | LEU  |
| 71  | O5    | 31  | LEU  |
| 71  | O5    | 43  | LYS  |
| 71  | O5    | 46  | THR  |
| 71  | O5    | 50  | SER  |
| 71  | O5    | 62  | GLN  |
| 71  | O5    | 71  | LYS  |
| 71  | O5    | 73  | LYS  |
| 71  | O5    | 74  | LYS  |
| 71  | O5    | 81  | ARG  |
| 71  | O5    | 84  | LYS  |
| 71  | O5    | 85  | THR  |
| 71  | O5    | 90  | ARG  |
| 71  | O5    | 94  | LYS  |
| 71  | O5    | 100 | VAL  |
| 71  | O5    | 101 | THR  |
| 71  | O5    | 104 | GLN  |
| 71  | O5    | 107 | LYS  |
| 71  | O5    | 115 | LYS  |
| 71  | O5    | 119 | LYS  |
| 72  | O6    | 11  | LEU  |
| 72  | O6    | 17  | VAL  |
| 72  | O6    | 18  | THR  |
| 72  | O6    | 21  | THR  |
| 72  | O6    | 25  | LYS  |
| 72  | O6    | 26  | ILE  |
| 72  | O6    | 36  | ARG  |
| 72  | O6    | 45  | ARG  |
| 72  | O6    | 57  | LEU  |
| 72  | O6    | 58  | ILE  |
| 72  | O6    | 60  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | O6    | 62  | ARG  |
| 72  | O6    | 64  | SER  |
| 72  | O6    | 68  | ARG  |
| 72  | O6    | 70  | ARG  |
| 72  | O6    | 72  | VAL  |
| 72  | O6    | 75  | LYS  |
| 72  | O6    | 76  | ARG  |
| 72  | O6    | 81  | THR  |
| 72  | O6    | 88  | GLU  |
| 72  | O6    | 89  | GLU  |
| 72  | O6    | 90  | MET  |
| 72  | O6    | 99  | ARG  |
| 73  | O7    | 5   | THR  |
| 73  | O7    | 17  | THR  |
| 73  | O7    | 24  | ARG  |
| 73  | O7    | 25  | ARG  |
| 73  | O7    | 31  | LYS  |
| 73  | O7    | 32  | LYS  |
| 73  | O7    | 33  | THR  |
| 73  | O7    | 45  | ARG  |
| 73  | O7    | 55  | ARG  |
| 73  | O7    | 58  | THR  |
| 73  | O7    | 59  | THR  |
| 73  | O7    | 67  | LEU  |
| 73  | O7    | 75  | LYS  |
| 73  | O7    | 82  | SER  |
| 73  | O7    | 84  | SER  |
| 74  | O8    | 5   | ILE  |
| 74  | O8    | 8   | ILE  |
| 74  | O8    | 12  | LEU  |
| 74  | O8    | 24  | THR  |
| 74  | O8    | 32  | ASN  |
| 74  | O8    | 45  | VAL  |
| 74  | O8    | 46  | ARG  |
| 74  | O8    | 53  | THR  |
| 74  | O8    | 54  | LEU  |
| 74  | O8    | 64  | LYS  |
| 74  | O8    | 65  | LEU  |
| 74  | O8    | 67  | GLN  |
| 74  | O8    | 77  | ARG  |
| 74  | O8    | 78  | LEU  |
| 75  | O9    | 4   | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | O9    | 5   | LYS  |
| 75  | O9    | 21  | ARG  |
| 75  | O9    | 23  | LEU  |
| 75  | O9    | 27  | ILE  |
| 75  | O9    | 30  | ARG  |
| 75  | O9    | 34  | THR  |
| 75  | O9    | 36  | ARG  |
| 75  | O9    | 45  | ARG  |
| 75  | O9    | 51  | ILE  |
| 76  | Q0    | 78  | ILE  |
| 76  | Q0    | 80  | PRO  |
| 76  | Q0    | 83  | LYS  |
| 76  | Q0    | 85  | LEU  |
| 76  | Q0    | 106 | ARG  |
| 76  | Q0    | 112 | LYS  |
| 76  | Q0    | 113 | ARG  |
| 76  | Q0    | 114 | LYS  |
| 76  | Q0    | 127 | LEU  |
| 77  | Q1    | 2   | ARG  |
| 77  | Q1    | 4   | LYS  |
| 77  | Q1    | 9   | ARG  |
| 77  | Q1    | 10  | THR  |
| 77  | Q1    | 11  | ARG  |
| 77  | Q1    | 13  | LEU  |
| 77  | Q1    | 15  | ARG  |
| 77  | Q1    | 19  | LYS  |
| 78  | Q2    | 2   | VAL  |
| 78  | Q2    | 3   | ASN  |
| 78  | Q2    | 4   | VAL  |
| 78  | Q2    | 8   | ARG  |
| 78  | Q2    | 16  | THR  |
| 78  | Q2    | 29  | LYS  |
| 78  | Q2    | 35  | LEU  |
| 78  | Q2    | 45  | ARG  |
| 78  | Q2    | 47  | GLN  |
| 78  | Q2    | 60  | LYS  |
| 78  | Q2    | 78  | LYS  |
| 78  | Q2    | 79  | THR  |
| 78  | Q2    | 80  | ARG  |
| 78  | Q2    | 83  | LEU  |
| 78  | Q2    | 84  | THR  |
| 78  | Q2    | 85  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | Q2    | 89  | LYS  |
| 78  | Q2    | 93  | LEU  |
| 78  | Q2    | 104 | LEU  |
| 79  | Q3    | 7   | LYS  |
| 79  | Q3    | 11  | THR  |
| 79  | Q3    | 16  | VAL  |
| 79  | Q3    | 25  | GLN  |
| 79  | Q3    | 26  | VAL  |
| 79  | Q3    | 31  | ILE  |
| 79  | Q3    | 45  | LYS  |
| 79  | Q3    | 46  | THR  |
| 79  | Q3    | 48  | LYS  |
| 79  | Q3    | 49  | ARG  |
| 79  | Q3    | 54  | ILE  |
| 79  | Q3    | 56  | THR  |
| 79  | Q3    | 60  | CYS  |
| 79  | Q3    | 78  | THR  |
| 79  | Q3    | 80  | ARG  |
| 79  | Q3    | 91  | GLU  |
| 2   | s0    | 6   | THR  |
| 2   | s0    | 9   | LEU  |
| 2   | s0    | 10  | THR  |
| 2   | s0    | 12  | GLU  |
| 2   | s0    | 28  | ASN  |
| 2   | s0    | 30  | GLN  |
| 2   | s0    | 31  | VAL  |
| 2   | s0    | 41  | ARG  |
| 2   | s0    | 45  | VAL  |
| 2   | s0    | 59  | LEU  |
| 2   | s0    | 62  | ARG  |
| 2   | s0    | 72  | ASP  |
| 2   | s0    | 80  | THR  |
| 2   | s0    | 87  | LEU  |
| 2   | s0    | 96  | THR  |
| 2   | s0    | 103 | THR  |
| 2   | s0    | 111 | ILE  |
| 2   | s0    | 112 | THR  |
| 2   | s0    | 119 | ARG  |
| 2   | s0    | 124 | THR  |
| 2   | s0    | 131 | GLN  |
| 2   | s0    | 144 | ILE  |
| 2   | s0    | 146 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | s0    | 153 | SER  |
| 2   | s0    | 157 | ASP  |
| 2   | s0    | 164 | ASN  |
| 2   | s0    | 167 | LYS  |
| 2   | s0    | 168 | HIS  |
| 2   | s0    | 172 | LEU  |
| 2   | s0    | 179 | ARG  |
| 2   | s0    | 183 | ARG  |
| 2   | s0    | 185 | ARG  |
| 2   | s0    | 188 | LEU  |
| 2   | s0    | 189 | VAL  |
| 2   | s0    | 191 | ARG  |
| 2   | s0    | 198 | MET  |
| 3   | s1    | 21  | VAL  |
| 3   | s1    | 25  | THR  |
| 3   | s1    | 47  | LEU  |
| 3   | s1    | 51  | SER  |
| 3   | s1    | 61  | LEU  |
| 3   | s1    | 62  | LYS  |
| 3   | s1    | 65  | VAL  |
| 3   | s1    | 66  | VAL  |
| 3   | s1    | 70  | LEU  |
| 3   | s1    | 73  | LEU  |
| 3   | s1    | 76  | SER  |
| 3   | s1    | 80  | SER  |
| 3   | s1    | 81  | PHE  |
| 3   | s1    | 89  | ASP  |
| 3   | s1    | 90  | GLU  |
| 3   | s1    | 96  | LEU  |
| 3   | s1    | 105 | PHE  |
| 3   | s1    | 111 | ARG  |
| 3   | s1    | 125 | VAL  |
| 3   | s1    | 126 | THR  |
| 3   | s1    | 127 | VAL  |
| 3   | s1    | 170 | GLU  |
| 3   | s1    | 173 | THR  |
| 3   | s1    | 177 | GLN  |
| 3   | s1    | 180 | THR  |
| 3   | s1    | 184 | LEU  |
| 3   | s1    | 192 | VAL  |
| 3   | s1    | 193 | ILE  |
| 3   | s1    | 197 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | s1    | 202 | LYS  |
| 3   | s1    | 203 | ASP  |
| 3   | s1    | 204 | ILE  |
| 3   | s1    | 212 | VAL  |
| 3   | s1    | 215 | VAL  |
| 3   | s1    | 217 | LEU  |
| 3   | s1    | 225 | VAL  |
| 3   | s1    | 228 | LEU  |
| 4   | s2    | 41  | LEU  |
| 4   | s2    | 53  | ILE  |
| 4   | s2    | 54  | GLU  |
| 4   | s2    | 55  | GLU  |
| 4   | s2    | 58  | LEU  |
| 4   | s2    | 69  | ILE  |
| 4   | s2    | 71  | THR  |
| 4   | s2    | 72  | LEU  |
| 4   | s2    | 77  | GLN  |
| 4   | s2    | 80  | VAL  |
| 4   | s2    | 83  | ILE  |
| 4   | s2    | 87  | GLN  |
| 4   | s2    | 89  | GLN  |
| 4   | s2    | 90  | THR  |
| 4   | s2    | 91  | ARG  |
| 4   | s2    | 97  | ARG  |
| 4   | s2    | 106 | ASP  |
| 4   | s2    | 111 | VAL  |
| 4   | s2    | 113 | LEU  |
| 4   | s2    | 117 | THR  |
| 4   | s2    | 130 | ILE  |
| 4   | s2    | 139 | ILE  |
| 4   | s2    | 140 | ARG  |
| 4   | s2    | 141 | ARG  |
| 4   | s2    | 146 | THR  |
| 4   | s2    | 148 | LEU  |
| 4   | s2    | 150 | GLN  |
| 4   | s2    | 159 | THR  |
| 4   | s2    | 185 | LYS  |
| 4   | s2    | 194 | GLU  |
| 4   | s2    | 200 | SER  |
| 4   | s2    | 205 | ARG  |
| 4   | s2    | 206 | THR  |
| 4   | s2    | 207 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | s2    | 218 | ILE  |
| 4   | s2    | 222 | TYR  |
| 4   | s2    | 225 | LEU  |
| 4   | s2    | 233 | GLN  |
| 4   | s2    | 242 | ILE  |
| 4   | s2    | 246 | GLU  |
| 5   | s3    | 4   | LEU  |
| 5   | s3    | 7   | LYS  |
| 5   | s3    | 9   | ARG  |
| 5   | s3    | 10  | LYS  |
| 5   | s3    | 11  | LEU  |
| 5   | s3    | 37  | VAL  |
| 5   | s3    | 39  | VAL  |
| 5   | s3    | 40  | ARG  |
| 5   | s3    | 41  | VAL  |
| 5   | s3    | 59  | LEU  |
| 5   | s3    | 66  | ILE  |
| 5   | s3    | 69  | LEU  |
| 5   | s3    | 84  | ILE  |
| 5   | s3    | 89  | GLU  |
| 5   | s3    | 92  | GLN  |
| 5   | s3    | 93  | ASP  |
| 5   | s3    | 94  | ARG  |
| 5   | s3    | 111 | ASN  |
| 5   | s3    | 115 | ILE  |
| 5   | s3    | 128 | GLU  |
| 5   | s3    | 132 | LYS  |
| 5   | s3    | 142 | LEU  |
| 5   | s3    | 143 | ARG  |
| 5   | s3    | 158 | ILE  |
| 5   | s3    | 162 | GLN  |
| 5   | s3    | 164 | VAL  |
| 5   | s3    | 168 | ILE  |
| 5   | s3    | 169 | ASP  |
| 5   | s3    | 172 | THR  |
| 5   | s3    | 175 | VAL  |
| 5   | s3    | 181 | VAL  |
| 5   | s3    | 185 | LYS  |
| 5   | s3    | 202 | LEU  |
| 5   | s3    | 212 | LYS  |
| 5   | s3    | 222 | VAL  |
| 5   | s3    | 223 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | s3    | 225 | TYR  |
| 6   | s4    | 7   | LYS  |
| 6   | s4    | 9   | LEU  |
| 6   | s4    | 23  | LEU  |
| 6   | s4    | 37  | LYS  |
| 6   | s4    | 38  | LEU  |
| 6   | s4    | 42  | LEU  |
| 6   | s4    | 48  | LEU  |
| 6   | s4    | 49  | ARG  |
| 6   | s4    | 51  | ARG  |
| 6   | s4    | 67  | GLN  |
| 6   | s4    | 70  | VAL  |
| 6   | s4    | 78  | THR  |
| 6   | s4    | 91  | THR  |
| 6   | s4    | 95  | THR  |
| 6   | s4    | 102 | VAL  |
| 6   | s4    | 105 | VAL  |
| 6   | s4    | 113 | ARG  |
| 6   | s4    | 116 | ASP  |
| 6   | s4    | 123 | LEU  |
| 6   | s4    | 126 | VAL  |
| 6   | s4    | 127 | LYS  |
| 6   | s4    | 129 | VAL  |
| 6   | s4    | 131 | LEU  |
| 6   | s4    | 147 | ILE  |
| 6   | s4    | 148 | ARG  |
| 6   | s4    | 160 | VAL  |
| 6   | s4    | 173 | ILE  |
| 6   | s4    | 180 | LEU  |
| 6   | s4    | 181 | VAL  |
| 6   | s4    | 182 | TYR  |
| 6   | s4    | 187 | ARG  |
| 6   | s4    | 191 | ARG  |
| 6   | s4    | 192 | ILE  |
| 6   | s4    | 208 | VAL  |
| 6   | s4    | 221 | ARG  |
| 6   | s4    | 222 | LEU  |
| 6   | s4    | 227 | VAL  |
| 6   | s4    | 236 | ILE  |
| 6   | s4    | 237 | SER  |
| 6   | s4    | 254 | ARG  |
| 7   | s5    | 23  | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | s5    | 24  | VAL  |
| 7   | s5    | 25  | LEU  |
| 7   | s5    | 27  | THR  |
| 7   | s5    | 32  | GLU  |
| 7   | s5    | 38  | THR  |
| 7   | s5    | 39  | GLU  |
| 7   | s5    | 45  | LYS  |
| 7   | s5    | 59  | VAL  |
| 7   | s5    | 63  | GLN  |
| 7   | s5    | 64  | VAL  |
| 7   | s5    | 66  | GLN  |
| 7   | s5    | 68  | ILE  |
| 7   | s5    | 76  | ARG  |
| 7   | s5    | 79  | ASN  |
| 7   | s5    | 83  | ARG  |
| 7   | s5    | 84  | LYS  |
| 7   | s5    | 89  | ILE  |
| 7   | s5    | 92  | ARG  |
| 7   | s5    | 93  | LEU  |
| 7   | s5    | 99  | MET  |
| 7   | s5    | 109 | LYS  |
| 7   | s5    | 112 | ARG  |
| 7   | s5    | 114 | ILE  |
| 7   | s5    | 119 | ASP  |
| 7   | s5    | 125 | THR  |
| 7   | s5    | 130 | ILE  |
| 7   | s5    | 146 | THR  |
| 7   | s5    | 147 | THR  |
| 7   | s5    | 148 | ARG  |
| 7   | s5    | 149 | VAL  |
| 7   | s5    | 157 | ARG  |
| 7   | s5    | 162 | VAL  |
| 7   | s5    | 163 | SER  |
| 7   | s5    | 167 | ARG  |
| 7   | s5    | 187 | ILE  |
| 7   | s5    | 194 | LEU  |
| 7   | s5    | 203 | LYS  |
| 7   | s5    | 216 | GLU  |
| 8   | s6    | 5   | ILE  |
| 8   | s6    | 17  | GLU  |
| 8   | s6    | 25  | ARG  |
| 8   | s6    | 30  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | s6    | 31  | ARG  |
| 8   | s6    | 44  | GLU  |
| 8   | s6    | 73  | ILE  |
| 8   | s6    | 76  | LEU  |
| 8   | s6    | 78  | THR  |
| 8   | s6    | 97  | VAL  |
| 8   | s6    | 98  | ARG  |
| 8   | s6    | 108 | VAL  |
| 8   | s6    | 109 | LEU  |
| 8   | s6    | 112 | VAL  |
| 8   | s6    | 115 | LYS  |
| 8   | s6    | 116 | LYS  |
| 8   | s6    | 120 | GLU  |
| 8   | s6    | 121 | LEU  |
| 8   | s6    | 125 | THR  |
| 8   | s6    | 126 | ASP  |
| 8   | s6    | 127 | THR  |
| 8   | s6    | 128 | THR  |
| 8   | s6    | 129 | VAL  |
| 8   | s6    | 143 | LYS  |
| 8   | s6    | 150 | GLU  |
| 8   | s6    | 151 | ASP  |
| 8   | s6    | 154 | ARG  |
| 8   | s6    | 155 | ASP  |
| 8   | s6    | 168 | THR  |
| 8   | s6    | 170 | THR  |
| 8   | s6    | 171 | LYS  |
| 8   | s6    | 177 | ARG  |
| 8   | s6    | 179 | VAL  |
| 8   | s6    | 193 | LEU  |
| 8   | s6    | 212 | LEU  |
| 8   | s6    | 215 | ARG  |
| 8   | s6    | 217 | SER  |
| 9   | s7    | 5   | GLN  |
| 9   | s7    | 8   | ILE  |
| 9   | s7    | 9   | LEU  |
| 9   | s7    | 19  | GLN  |
| 9   | s7    | 26  | GLU  |
| 9   | s7    | 28  | GLU  |
| 9   | s7    | 33  | GLU  |
| 9   | s7    | 49  | ILE  |
| 9   | s7    | 50  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | s7    | 55  | LYS  |
| 9   | s7    | 62  | VAL  |
| 9   | s7    | 67  | LEU  |
| 9   | s7    | 77  | LEU  |
| 9   | s7    | 79  | ARG  |
| 9   | s7    | 80  | GLU  |
| 9   | s7    | 86  | GLN  |
| 9   | s7    | 95  | GLU  |
| 9   | s7    | 97  | ARG  |
| 9   | s7    | 101 | LYS  |
| 9   | s7    | 105 | THR  |
| 9   | s7    | 110 | GLN  |
| 9   | s7    | 114 | ARG  |
| 9   | s7    | 116 | ARG  |
| 9   | s7    | 117 | THR  |
| 9   | s7    | 118 | LEU  |
| 9   | s7    | 126 | LEU  |
| 9   | s7    | 136 | VAL  |
| 9   | s7    | 143 | LEU  |
| 9   | s7    | 144 | VAL  |
| 9   | s7    | 148 | LYS  |
| 9   | s7    | 149 | ILE  |
| 9   | s7    | 150 | GLN  |
| 9   | s7    | 156 | SER  |
| 9   | s7    | 159 | VAL  |
| 9   | s7    | 160 | GLN  |
| 9   | s7    | 166 | LEU  |
| 9   | s7    | 175 | LYS  |
| 9   | s7    | 185 | ILE  |
| 10  | s8    | 18  | ARG  |
| 10  | s8    | 25  | ARG  |
| 10  | s8    | 26  | LYS  |
| 10  | s8    | 29  | LEU  |
| 10  | s8    | 36  | THR  |
| 10  | s8    | 46  | VAL  |
| 10  | s8    | 60  | ILE  |
| 10  | s8    | 61  | GLU  |
| 10  | s8    | 74  | LYS  |
| 10  | s8    | 76  | THR  |
| 10  | s8    | 77  | ARG  |
| 10  | s8    | 89  | GLU  |
| 10  | s8    | 119 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | s8    | 121 | LEU  |
| 10  | s8    | 123 | LYS  |
| 10  | s8    | 138 | ASN  |
| 10  | s8    | 151 | LYS  |
| 10  | s8    | 154 | SER  |
| 10  | s8    | 155 | SER  |
| 10  | s8    | 158 | SER  |
| 10  | s8    | 183 | ILE  |
| 10  | s8    | 184 | LEU  |
| 10  | s8    | 199 | LYS  |
| 11  | s9    | 3   | ARG  |
| 11  | s9    | 6   | ARG  |
| 11  | s9    | 7   | THR  |
| 11  | s9    | 10  | LYS  |
| 11  | s9    | 16  | LYS  |
| 11  | s9    | 28  | LEU  |
| 11  | s9    | 33  | GLU  |
| 11  | s9    | 37  | LYS  |
| 11  | s9    | 39  | LYS  |
| 11  | s9    | 40  | LYS  |
| 11  | s9    | 49  | LEU  |
| 11  | s9    | 82  | ARG  |
| 11  | s9    | 93  | LEU  |
| 11  | s9    | 96  | VAL  |
| 11  | s9    | 99  | LEU  |
| 11  | s9    | 101 | VAL  |
| 11  | s9    | 105 | LEU  |
| 11  | s9    | 109 | LEU  |
| 11  | s9    | 110 | GLN  |
| 11  | s9    | 111 | THR  |
| 11  | s9    | 113 | VAL  |
| 11  | s9    | 118 | LEU  |
| 11  | s9    | 130 | THR  |
| 11  | s9    | 134 | ILE  |
| 11  | s9    | 140 | ILE  |
| 11  | s9    | 149 | ARG  |
| 11  | s9    | 154 | LYS  |
| 11  | s9    | 161 | THR  |
| 11  | s9    | 168 | ARG  |
| 11  | s9    | 172 | VAL  |
| 11  | s9    | 182 | GLU  |
| 12  | c0    | 2   | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | c0    | 5   | LYS  |
| 12  | c0    | 15  | LEU  |
| 12  | c0    | 20  | VAL  |
| 12  | c0    | 21  | VAL  |
| 12  | c0    | 27  | PHE  |
| 12  | c0    | 33  | GLU  |
| 12  | c0    | 34  | GLU  |
| 12  | c0    | 36  | ASP  |
| 12  | c0    | 55  | VAL  |
| 12  | c0    | 56  | LYS  |
| 12  | c0    | 57  | THR  |
| 12  | c0    | 67  | THR  |
| 12  | c0    | 71  | GLU  |
| 13  | c1    | 5   | LEU  |
| 13  | c1    | 10  | GLU  |
| 13  | c1    | 21  | ASN  |
| 13  | c1    | 26  | LYS  |
| 13  | c1    | 27  | THR  |
| 13  | c1    | 30  | ARG  |
| 13  | c1    | 32  | LYS  |
| 13  | c1    | 33  | ARG  |
| 13  | c1    | 40  | LEU  |
| 13  | c1    | 44  | THR  |
| 13  | c1    | 47  | THR  |
| 13  | c1    | 54  | ILE  |
| 13  | c1    | 56  | LYS  |
| 13  | c1    | 60  | PHE  |
| 13  | c1    | 64  | VAL  |
| 13  | c1    | 69  | LYS  |
| 13  | c1    | 74  | THR  |
| 13  | c1    | 80  | MET  |
| 13  | c1    | 83  | THR  |
| 13  | c1    | 109 | VAL  |
| 13  | c1    | 123 | VAL  |
| 13  | c1    | 129 | ARG  |
| 13  | c1    | 140 | VAL  |
| 13  | c1    | 143 | SER  |
| 14  | c2    | 28  | LEU  |
| 14  | c2    | 31  | VAL  |
| 14  | c2    | 37  | VAL  |
| 14  | c2    | 43  | ARG  |
| 14  | c2    | 45  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | c2    | 52  | LEU  |
| 14  | c2    | 53  | THR  |
| 14  | c2    | 58  | LEU  |
| 14  | c2    | 59  | LEU  |
| 14  | c2    | 61  | VAL  |
| 14  | c2    | 67  | THR  |
| 14  | c2    | 71  | ILE  |
| 14  | c2    | 74  | LEU  |
| 14  | c2    | 83  | GLU  |
| 14  | c2    | 85  | LYS  |
| 14  | c2    | 86  | VAL  |
| 14  | c2    | 89  | ILE  |
| 14  | c2    | 103 | LEU  |
| 14  | c2    | 116 | VAL  |
| 14  | c2    | 120 | VAL  |
| 14  | c2    | 121 | VAL  |
| 14  | c2    | 132 | GLU  |
| 14  | c2    | 137 | MET  |
| 14  | c2    | 138 | GLU  |
| 14  | c2    | 140 | PHE  |
| 15  | c3    | 12  | SER  |
| 15  | c3    | 16  | ILE  |
| 15  | c3    | 20  | ARG  |
| 15  | c3    | 21  | ASN  |
| 15  | c3    | 39  | LYS  |
| 15  | c3    | 46  | THR  |
| 15  | c3    | 53  | LEU  |
| 15  | c3    | 66  | ILE  |
| 15  | c3    | 67  | THR  |
| 15  | c3    | 70  | LYS  |
| 15  | c3    | 76  | LYS  |
| 15  | c3    | 80  | LEU  |
| 15  | c3    | 87  | ASP  |
| 15  | c3    | 88  | LEU  |
| 15  | c3    | 93  | LYS  |
| 15  | c3    | 106 | ARG  |
| 15  | c3    | 114 | ARG  |
| 15  | c3    | 115 | LEU  |
| 15  | c3    | 125 | LEU  |
| 15  | c3    | 127 | ARG  |
| 15  | c3    | 131 | THR  |
| 15  | c3    | 134 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | c3    | 138 | ASN  |
| 15  | c3    | 147 | SER  |
| 15  | c3    | 150 | VAL  |
| 16  | c4    | 18  | ARG  |
| 16  | c4    | 26  | THR  |
| 16  | c4    | 33  | LEU  |
| 16  | c4    | 49  | LYS  |
| 16  | c4    | 51  | ASP  |
| 16  | c4    | 61  | MET  |
| 16  | c4    | 62  | LEU  |
| 16  | c4    | 70  | LYS  |
| 16  | c4    | 79  | VAL  |
| 16  | c4    | 81  | VAL  |
| 16  | c4    | 92  | LYS  |
| 16  | c4    | 102 | LEU  |
| 16  | c4    | 114 | ARG  |
| 16  | c4    | 119 | THR  |
| 16  | c4    | 125 | SER  |
| 16  | c4    | 127 | ARG  |
| 16  | c4    | 132 | ARG  |
| 16  | c4    | 133 | ARG  |
| 16  | c4    | 136 | ARG  |
| 16  | c4    | 137 | LEU  |
| 17  | c5    | 10  | ARG  |
| 17  | c5    | 11  | VAL  |
| 17  | c5    | 12  | PHE  |
| 17  | c5    | 22  | LEU  |
| 17  | c5    | 23  | GLU  |
| 17  | c5    | 24  | LYS  |
| 17  | c5    | 27  | GLU  |
| 17  | c5    | 36  | LEU  |
| 17  | c5    | 64  | LYS  |
| 17  | c5    | 69  | GLU  |
| 17  | c5    | 71  | GLU  |
| 17  | c5    | 72  | LYS  |
| 17  | c5    | 76  | VAL  |
| 17  | c5    | 77  | ARG  |
| 17  | c5    | 92  | SER  |
| 17  | c5    | 94  | VAL  |
| 17  | c5    | 107 | ILE  |
| 17  | c5    | 110 | GLU  |
| 17  | c5    | 122 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | c5    | 124 | THR  |
| 17  | c5    | 125 | PRO  |
| 18  | c6    | 7   | VAL  |
| 18  | c6    | 17  | THR  |
| 18  | c6    | 23  | LYS  |
| 18  | c6    | 28  | LEU  |
| 18  | c6    | 37  | THR  |
| 18  | c6    | 40  | GLU  |
| 18  | c6    | 43  | ILE  |
| 18  | c6    | 48  | VAL  |
| 18  | c6    | 53  | LEU  |
| 18  | c6    | 54  | LEU  |
| 18  | c6    | 57  | LEU  |
| 18  | c6    | 68  | ARG  |
| 18  | c6    | 69  | VAL  |
| 18  | c6    | 70  | THR  |
| 18  | c6    | 81  | ILE  |
| 18  | c6    | 90  | VAL  |
| 18  | c6    | 94  | GLN  |
| 18  | c6    | 110 | THR  |
| 18  | c6    | 113 | ASP  |
| 18  | c6    | 114 | ARG  |
| 18  | c6    | 137 | ARG  |
| 18  | c6    | 143 | ARG  |
| 19  | c7    | 5   | ARG  |
| 19  | c7    | 8   | THR  |
| 19  | c7    | 14  | LYS  |
| 19  | c7    | 33  | ARG  |
| 19  | c7    | 34  | LEU  |
| 19  | c7    | 38  | ILE  |
| 19  | c7    | 46  | LEU  |
| 19  | c7    | 55  | THR  |
| 19  | c7    | 60  | ARG  |
| 19  | c7    | 66  | VAL  |
| 19  | c7    | 72  | LYS  |
| 19  | c7    | 74  | GLN  |
| 19  | c7    | 83  | GLN  |
| 19  | c7    | 85  | VAL  |
| 19  | c7    | 104 | ASN  |
| 19  | c7    | 105 | GLN  |
| 19  | c7    | 110 | VAL  |
| 19  | c7    | 113 | LEU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | c8    | 2   | SER  |
| 20  | c8    | 3   | LEU  |
| 20  | c8    | 4   | VAL  |
| 20  | c8    | 5   | VAL  |
| 20  | c8    | 6   | GLN  |
| 20  | c8    | 13  | HIS  |
| 20  | c8    | 15  | LEU  |
| 20  | c8    | 16  | ARG  |
| 20  | c8    | 28  | ILE  |
| 20  | c8    | 34  | THR  |
| 20  | c8    | 36  | LYS  |
| 20  | c8    | 40  | ARG  |
| 20  | c8    | 46  | VAL  |
| 20  | c8    | 57  | ARG  |
| 20  | c8    | 61  | LEU  |
| 20  | c8    | 63  | GLN  |
| 20  | c8    | 68  | ARG  |
| 20  | c8    | 69  | ILE  |
| 20  | c8    | 80  | LYS  |
| 20  | c8    | 92  | ILE  |
| 20  | c8    | 100 | THR  |
| 20  | c8    | 105 | VAL  |
| 20  | c8    | 110 | ARG  |
| 20  | c8    | 113 | LEU  |
| 20  | c8    | 116 | LEU  |
| 20  | c8    | 119 | ILE  |
| 20  | c8    | 136 | GLN  |
| 20  | c8    | 138 | THR  |
| 20  | c8    | 143 | ARG  |
| 20  | c8    | 145 | ARG  |
| 21  | c9    | 6   | VAL  |
| 21  | c9    | 13  | ASP  |
| 21  | c9    | 25  | GLN  |
| 21  | c9    | 28  | LEU  |
| 21  | c9    | 30  | VAL  |
| 21  | c9    | 34  | VAL  |
| 21  | c9    | 36  | ILE  |
| 21  | c9    | 37  | VAL  |
| 21  | c9    | 38  | LYS  |
| 21  | c9    | 57  | ARG  |
| 21  | c9    | 68  | ARG  |
| 21  | c9    | 71  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | c9    | 86  | ARG  |
| 21  | c9    | 88  | VAL  |
| 21  | c9    | 110 | LYS  |
| 21  | c9    | 111 | ILE  |
| 21  | c9    | 116 | ILE  |
| 21  | c9    | 123 | ARG  |
| 21  | c9    | 131 | ASP  |
| 21  | c9    | 132 | LEU  |
| 21  | c9    | 135 | ILE  |
| 21  | c9    | 140 | LEU  |
| 21  | c9    | 142 | GLU  |
| 21  | c9    | 144 | GLU  |
| 22  | d0    | 12  | GLN  |
| 22  | d0    | 16  | GLN  |
| 22  | d0    | 20  | ILE  |
| 22  | d0    | 23  | ARG  |
| 22  | d0    | 27  | THR  |
| 22  | d0    | 30  | LYS  |
| 22  | d0    | 44  | ASN  |
| 22  | d0    | 47  | GLN  |
| 22  | d0    | 51  | VAL  |
| 22  | d0    | 57  | ARG  |
| 22  | d0    | 60  | THR  |
| 22  | d0    | 63  | LEU  |
| 22  | d0    | 67  | THR  |
| 22  | d0    | 70  | THR  |
| 22  | d0    | 72  | ASN  |
| 22  | d0    | 74  | GLU  |
| 22  | d0    | 81  | THR  |
| 22  | d0    | 88  | LYS  |
| 22  | d0    | 89  | ARG  |
| 22  | d0    | 97  | VAL  |
| 22  | d0    | 99  | ILE  |
| 22  | d0    | 102 | ARG  |
| 22  | d0    | 103 | ILE  |
| 22  | d0    | 107 | THR  |
| 22  | d0    | 108 | ILE  |
| 22  | d0    | 118 | VAL  |
| 23  | d1    | 1   | MET  |
| 23  | d1    | 2   | GLU  |
| 23  | d1    | 5   | LYS  |
| 23  | d1    | 10  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | d1    | 11  | LEU  |
| 23  | d1    | 12  | TYR  |
| 23  | d1    | 25  | LYS  |
| 23  | d1    | 32  | VAL  |
| 23  | d1    | 34  | ILE  |
| 23  | d1    | 38  | LYS  |
| 23  | d1    | 41  | GLU  |
| 23  | d1    | 44  | ARG  |
| 23  | d1    | 49  | GLU  |
| 23  | d1    | 52  | THR  |
| 23  | d1    | 62  | ARG  |
| 23  | d1    | 68  | SER  |
| 23  | d1    | 69  | LEU  |
| 23  | d1    | 74  | GLN  |
| 23  | d1    | 76  | ASP  |
| 23  | d1    | 79  | LEU  |
| 23  | d1    | 81  | ASN  |
| 24  | d2    | 6   | VAL  |
| 24  | d2    | 7   | LEU  |
| 24  | d2    | 22  | LYS  |
| 24  | d2    | 23  | ARG  |
| 24  | d2    | 25  | VAL  |
| 24  | d2    | 26  | LEU  |
| 24  | d2    | 43  | LYS  |
| 24  | d2    | 65  | LEU  |
| 24  | d2    | 68  | ARG  |
| 24  | d2    | 74  | VAL  |
| 24  | d2    | 88  | LYS  |
| 24  | d2    | 93  | LEU  |
| 24  | d2    | 103 | ILE  |
| 24  | d2    | 105 | THR  |
| 24  | d2    | 129 | VAL  |
| 25  | d3    | 3   | LYS  |
| 25  | d3    | 9   | LEU  |
| 25  | d3    | 16  | ARG  |
| 25  | d3    | 19  | ARG  |
| 25  | d3    | 23  | ARG  |
| 25  | d3    | 40  | SER  |
| 25  | d3    | 56  | LYS  |
| 25  | d3    | 69  | ARG  |
| 25  | d3    | 73  | ARG  |
| 25  | d3    | 83  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | d3    | 84  | THR  |
| 25  | d3    | 96  | VAL  |
| 25  | d3    | 98  | GLU  |
| 25  | d3    | 100 | ASP  |
| 25  | d3    | 103 | LEU  |
| 25  | d3    | 107 | PHE  |
| 25  | d3    | 112 | LYS  |
| 25  | d3    | 114 | LYS  |
| 25  | d3    | 117 | ILE  |
| 25  | d3    | 131 | SER  |
| 25  | d3    | 133 | LEU  |
| 26  | d4    | 5   | VAL  |
| 26  | d4    | 10  | ARG  |
| 26  | d4    | 13  | ILE  |
| 26  | d4    | 21  | LYS  |
| 26  | d4    | 34  | ASN  |
| 26  | d4    | 36  | SER  |
| 26  | d4    | 42  | GLU  |
| 26  | d4    | 43  | LYS  |
| 26  | d4    | 44  | LEU  |
| 26  | d4    | 46  | GLU  |
| 26  | d4    | 47  | VAL  |
| 26  | d4    | 49  | LYS  |
| 26  | d4    | 51  | GLU  |
| 26  | d4    | 55  | VAL  |
| 26  | d4    | 61  | ARG  |
| 26  | d4    | 62  | THR  |
| 26  | d4    | 88  | THR  |
| 26  | d4    | 100 | VAL  |
| 26  | d4    | 105 | ARG  |
| 26  | d4    | 114 | ARG  |
| 26  | d4    | 116 | LYS  |
| 27  | d5    | 43  | ASP  |
| 27  | d5    | 46  | LYS  |
| 27  | d5    | 51  | LEU  |
| 27  | d5    | 57  | TYR  |
| 27  | d5    | 60  | VAL  |
| 27  | d5    | 78  | ILE  |
| 27  | d5    | 81  | ARG  |
| 27  | d5    | 97  | LYS  |
| 28  | d6    | 12  | LYS  |
| 28  | d6    | 18  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | d6    | 24  | VAL  |
| 28  | d6    | 34  | LYS  |
| 28  | d6    | 41  | ILE  |
| 28  | d6    | 44  | ILE  |
| 28  | d6    | 53  | LEU  |
| 28  | d6    | 55  | GLU  |
| 28  | d6    | 83  | ILE  |
| 28  | d6    | 85  | ARG  |
| 28  | d6    | 90  | GLU  |
| 29  | d7    | 3   | LEU  |
| 29  | d7    | 40  | CYS  |
| 29  | d7    | 43  | ILE  |
| 29  | d7    | 44  | THR  |
| 29  | d7    | 52  | THR  |
| 29  | d7    | 61  | THR  |
| 29  | d7    | 63  | LEU  |
| 29  | d7    | 72  | LYS  |
| 29  | d7    | 77  | THR  |
| 29  | d7    | 81  | ARG  |
| 29  | d7    | 82  | LYS  |
| 30  | d8    | 7   | VAL  |
| 30  | d8    | 8   | THR  |
| 30  | d8    | 16  | LEU  |
| 30  | d8    | 22  | ARG  |
| 30  | d8    | 33  | LEU  |
| 30  | d8    | 36  | THR  |
| 30  | d8    | 40  | ILE  |
| 30  | d8    | 48  | VAL  |
| 30  | d8    | 49  | ARG  |
| 30  | d8    | 54  | LEU  |
| 31  | d9    | 10  | HIS  |
| 31  | d9    | 16  | LYS  |
| 31  | d9    | 28  | THR  |
| 31  | d9    | 30  | LEU  |
| 31  | d9    | 31  | ILE  |
| 31  | d9    | 32  | ARG  |
| 31  | d9    | 36  | LEU  |
| 31  | d9    | 38  | ILE  |
| 31  | d9    | 53  | ASN  |
| 31  | d9    | 54  | LYS  |
| 80  | e0    | 4   | VAL  |
| 80  | e0    | 13  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 80  | e0    | 21  | VAL  |
| 80  | e0    | 22  | GLU  |
| 80  | e0    | 23  | LYS  |
| 80  | e0    | 26  | LYS  |
| 80  | e0    | 29  | LYS  |
| 80  | e0    | 36  | LYS  |
| 80  | e0    | 38  | LEU  |
| 80  | e0    | 46  | ASN  |
| 80  | e0    | 49  | LEU  |
| 80  | e0    | 54  | ARG  |
| 80  | e0    | 55  | ARG  |
| 33  | e1    | 80  | ARG  |
| 33  | e1    | 84  | VAL  |
| 33  | e1    | 86  | THR  |
| 33  | e1    | 96  | LYS  |
| 33  | e1    | 100 | LEU  |
| 33  | e1    | 102 | VAL  |
| 33  | e1    | 106 | TYR  |
| 33  | e1    | 113 | LYS  |
| 33  | e1    | 119 | ARG  |
| 33  | e1    | 120 | GLU  |
| 33  | e1    | 121 | CYS  |
| 33  | e1    | 125 | THR  |
| 33  | e1    | 130 | VAL  |
| 33  | e1    | 135 | HIS  |
| 33  | e1    | 137 | ASP  |
| 33  | e1    | 146 | SER  |
| 33  | e1    | 147 | VAL  |
| 33  | e1    | 148 | TYR  |
| 33  | e1    | 150 | VAL  |
| 34  | sR    | 8   | VAL  |
| 34  | sR    | 21  | THR  |
| 34  | sR    | 23  | LEU  |
| 34  | sR    | 25  | THR  |
| 34  | sR    | 29  | GLN  |
| 34  | sR    | 58  | VAL  |
| 34  | sR    | 65  | SER  |
| 34  | sR    | 76  | ASP  |
| 34  | sR    | 96  | THR  |
| 34  | sR    | 106 | HIS  |
| 34  | sR    | 118 | LYS  |
| 34  | sR    | 136 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | sR    | 145 | LEU  |
| 34  | sR    | 159 | ASN  |
| 34  | sR    | 166 | SER  |
| 34  | sR    | 168 | THR  |
| 34  | sR    | 184 | ASN  |
| 34  | sR    | 199 | ILE  |
| 34  | sR    | 202 | LEU  |
| 34  | sR    | 228 | LYS  |
| 34  | sR    | 252 | LEU  |
| 34  | sR    | 266 | ASP  |
| 34  | sR    | 275 | ARG  |
| 34  | sR    | 309 | VAL  |
| 34  | sR    | 314 | GLN  |
| 34  | sR    | 317 | THR  |
| 35  | sM    | 23  | LYS  |
| 35  | sM    | 25  | ILE  |
| 35  | sM    | 33  | LYS  |
| 35  | sM    | 43  | ASP  |
| 35  | sM    | 45  | SER  |
| 35  | sM    | 64  | LYS  |
| 35  | sM    | 74  | LYS  |
| 35  | sM    | 75  | ASP  |
| 39  | l2    | 15  | ILE  |
| 39  | l2    | 23  | ARG  |
| 39  | l2    | 32  | LEU  |
| 39  | l2    | 41  | ILE  |
| 39  | l2    | 44  | ILE  |
| 39  | l2    | 45  | VAL  |
| 39  | l2    | 46  | LYS  |
| 39  | l2    | 48  | ILE  |
| 39  | l2    | 60  | LYS  |
| 39  | l2    | 61  | VAL  |
| 39  | l2    | 62  | VAL  |
| 39  | l2    | 68  | LYS  |
| 39  | l2    | 70  | ARG  |
| 39  | l2    | 71  | LEU  |
| 39  | l2    | 74  | GLU  |
| 39  | l2    | 77  | ILE  |
| 39  | l2    | 82  | VAL  |
| 39  | l2    | 101 | VAL  |
| 39  | l2    | 109 | GLU  |
| 39  | l2    | 112 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | l2    | 116 | VAL  |
| 39  | l2    | 119 | LYS  |
| 39  | l2    | 134 | VAL  |
| 39  | l2    | 136 | ILE  |
| 39  | l2    | 137 | ILE  |
| 39  | l2    | 142 | ASP  |
| 39  | l2    | 155 | LYS  |
| 39  | l2    | 157 | VAL  |
| 39  | l2    | 158 | ILE  |
| 39  | l2    | 165 | VAL  |
| 39  | l2    | 168 | VAL  |
| 39  | l2    | 169 | ILE  |
| 39  | l2    | 179 | LEU  |
| 39  | l2    | 180 | LEU  |
| 39  | l2    | 181 | LYS  |
| 39  | l2    | 193 | ARG  |
| 39  | l2    | 202 | VAL  |
| 39  | l2    | 207 | VAL  |
| 39  | l2    | 208 | ASP  |
| 39  | l2    | 215 | ASN  |
| 39  | l2    | 224 | THR  |
| 39  | l2    | 225 | ILE  |
| 39  | l2    | 230 | VAL  |
| 39  | l2    | 241 | ARG  |
| 39  | l2    | 246 | LEU  |
| 39  | l2    | 249 | SER  |
| 40  | l3    | 3   | HIS  |
| 40  | l3    | 4   | ARG  |
| 40  | l3    | 10  | ARG  |
| 40  | l3    | 17  | LEU  |
| 40  | l3    | 19  | ARG  |
| 40  | l3    | 21  | ARG  |
| 40  | l3    | 30  | LYS  |
| 40  | l3    | 37  | ARG  |
| 40  | l3    | 39  | LYS  |
| 40  | l3    | 43  | LEU  |
| 40  | l3    | 47  | LEU  |
| 40  | l3    | 50  | LYS  |
| 40  | l3    | 56  | ILE  |
| 40  | l3    | 69  | LYS  |
| 40  | l3    | 73  | VAL  |
| 40  | l3    | 77  | THR  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | l3    | 79  | VAL  |
| 40  | l3    | 81  | THR  |
| 40  | l3    | 84  | VAL  |
| 40  | l3    | 85  | VAL  |
| 40  | l3    | 103 | THR  |
| 40  | l3    | 114 | VAL  |
| 40  | l3    | 120 | LYS  |
| 40  | l3    | 124 | LYS  |
| 40  | l3    | 134 | SER  |
| 40  | l3    | 145 | GLU  |
| 40  | l3    | 148 | LEU  |
| 40  | l3    | 150 | ARG  |
| 40  | l3    | 157 | VAL  |
| 40  | l3    | 160 | VAL  |
| 40  | l3    | 169 | THR  |
| 40  | l3    | 183 | LEU  |
| 40  | l3    | 187 | SER  |
| 40  | l3    | 188 | ILE  |
| 40  | l3    | 192 | VAL  |
| 40  | l3    | 196 | ARG  |
| 40  | l3    | 201 | LYS  |
| 40  | l3    | 202 | THR  |
| 40  | l3    | 205 | VAL  |
| 40  | l3    | 221 | THR  |
| 40  | l3    | 229 | VAL  |
| 40  | l3    | 232 | ARG  |
| 40  | l3    | 235 | THR  |
| 40  | l3    | 236 | LYS  |
| 40  | l3    | 238 | LEU  |
| 40  | l3    | 242 | THR  |
| 40  | l3    | 248 | LYS  |
| 40  | l3    | 249 | VAL  |
| 40  | l3    | 252 | ILE  |
| 40  | l3    | 261 | MET  |
| 40  | l3    | 264 | VAL  |
| 40  | l3    | 275 | ARG  |
| 40  | l3    | 284 | ARG  |
| 40  | l3    | 287 | LYS  |
| 40  | l3    | 296 | THR  |
| 40  | l3    | 302 | LYS  |
| 40  | l3    | 308 | MET  |
| 40  | l3    | 317 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | l3    | 318 | LYS  |
| 40  | l3    | 324 | VAL  |
| 40  | l3    | 328 | ILE  |
| 40  | l3    | 335 | ILE  |
| 40  | l3    | 338 | LEU  |
| 40  | l3    | 340 | LYS  |
| 40  | l3    | 346 | THR  |
| 40  | l3    | 347 | SER  |
| 40  | l3    | 348 | ARG  |
| 40  | l3    | 349 | LYS  |
| 40  | l3    | 354 | VAL  |
| 40  | l3    | 355 | SER  |
| 40  | l3    | 361 | THR  |
| 40  | l3    | 367 | LYS  |
| 40  | l3    | 380 | MET  |
| 40  | l3    | 382 | THR  |
| 41  | l4    | 2   | SER  |
| 41  | l4    | 3   | ARG  |
| 41  | l4    | 14  | GLU  |
| 41  | l4    | 16  | THR  |
| 41  | l4    | 25  | VAL  |
| 41  | l4    | 47  | ARG  |
| 41  | l4    | 52  | VAL  |
| 41  | l4    | 60  | THR  |
| 41  | l4    | 67  | THR  |
| 41  | l4    | 69  | ARG  |
| 41  | l4    | 71  | VAL  |
| 41  | l4    | 93  | MET  |
| 41  | l4    | 112 | LYS  |
| 41  | l4    | 122 | THR  |
| 41  | l4    | 143 | GLU  |
| 41  | l4    | 144 | LYS  |
| 41  | l4    | 145 | ILE  |
| 41  | l4    | 150 | LEU  |
| 41  | l4    | 156 | LEU  |
| 41  | l4    | 160 | GLN  |
| 41  | l4    | 161 | LYS  |
| 41  | l4    | 172 | VAL  |
| 41  | l4    | 179 | LEU  |
| 41  | l4    | 185 | LYS  |
| 41  | l4    | 186 | LYS  |
| 41  | l4    | 187 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | l4    | 188 | ARG  |
| 41  | l4    | 191 | LYS  |
| 41  | l4    | 193 | LYS  |
| 41  | l4    | 198 | ARG  |
| 41  | l4    | 200 | THR  |
| 41  | l4    | 203 | ARG  |
| 41  | l4    | 206 | LEU  |
| 41  | l4    | 217 | LYS  |
| 41  | l4    | 220 | ARG  |
| 41  | l4    | 222 | VAL  |
| 41  | l4    | 226 | GLU  |
| 41  | l4    | 229 | ASN  |
| 41  | l4    | 230 | VAL  |
| 41  | l4    | 246 | ARG  |
| 41  | l4    | 258 | LEU  |
| 41  | l4    | 267 | VAL  |
| 41  | l4    | 283 | THR  |
| 41  | l4    | 284 | SER  |
| 41  | l4    | 287 | THR  |
| 41  | l4    | 295 | ILE  |
| 41  | l4    | 300 | ARG  |
| 41  | l4    | 306 | THR  |
| 41  | l4    | 307 | GLN  |
| 41  | l4    | 313 | LEU  |
| 41  | l4    | 319 | LYS  |
| 41  | l4    | 323 | VAL  |
| 41  | l4    | 327 | LEU  |
| 41  | l4    | 333 | VAL  |
| 41  | l4    | 342 | LYS  |
| 41  | l4    | 345 | GLU  |
| 41  | l4    | 357 | GLU  |
| 41  | l4    | 358 | THR  |
| 41  | l4    | 359 | LEU  |
| 41  | l4    | 360 | LYS  |
| 42  | l5    | 4   | GLN  |
| 42  | l5    | 5   | LYS  |
| 42  | l5    | 15  | ARG  |
| 42  | l5    | 34  | LYS  |
| 42  | l5    | 35  | ARG  |
| 42  | l5    | 41  | LYS  |
| 42  | l5    | 45  | ASN  |
| 42  | l5    | 51  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | 15    | 58  | LYS  |
| 42  | 15    | 61  | ILE  |
| 42  | 15    | 65  | ILE  |
| 42  | 15    | 68  | THR  |
| 42  | 15    | 70  | THR  |
| 42  | 15    | 73  | VAL  |
| 42  | 15    | 74  | VAL  |
| 42  | 15    | 75  | LEU  |
| 42  | 15    | 89  | THR  |
| 42  | 15    | 93  | THR  |
| 42  | 15    | 109 | THR  |
| 42  | 15    | 110 | LEU  |
| 42  | 15    | 112 | LYS  |
| 42  | 15    | 113 | LEU  |
| 42  | 15    | 115 | LEU  |
| 42  | 15    | 118 | THR  |
| 42  | 15    | 120 | LYS  |
| 42  | 15    | 124 | GLU  |
| 42  | 15    | 131 | LEU  |
| 42  | 15    | 132 | THR  |
| 42  | 15    | 133 | GLU  |
| 42  | 15    | 135 | VAL  |
| 42  | 15    | 136 | GLU  |
| 42  | 15    | 140 | ARG  |
| 42  | 15    | 144 | VAL  |
| 42  | 15    | 146 | LEU  |
| 42  | 15    | 148 | ILE  |
| 42  | 15    | 152 | ARG  |
| 42  | 15    | 155 | THR  |
| 42  | 15    | 158 | ARG  |
| 42  | 15    | 163 | LEU  |
| 42  | 15    | 173 | VAL  |
| 42  | 15    | 177 | GLU  |
| 42  | 15    | 185 | PHE  |
| 42  | 15    | 187 | THR  |
| 42  | 15    | 189 | GLU  |
| 42  | 15    | 190 | ILE  |
| 42  | 15    | 194 | LEU  |
| 42  | 15    | 210 | GLU  |
| 42  | 15    | 211 | LEU  |
| 42  | 15    | 218 | ARG  |
| 42  | 15    | 220 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | 15    | 227 | LEU  |
| 42  | 15    | 254 | LYS  |
| 42  | 15    | 257 | GLU  |
| 42  | 15    | 258 | LYS  |
| 42  | 15    | 259 | LYS  |
| 42  | 15    | 268 | GLU  |
| 42  | 15    | 271 | LYS  |
| 42  | 15    | 273 | ARG  |
| 42  | 15    | 275 | THR  |
| 42  | 15    | 293 | LEU  |
| 43  | 16    | 8   | LYS  |
| 43  | 16    | 12  | SER  |
| 43  | 16    | 20  | LYS  |
| 43  | 16    | 21  | THR  |
| 43  | 16    | 31  | ARG  |
| 43  | 16    | 46  | ARG  |
| 43  | 16    | 50  | LYS  |
| 43  | 16    | 52  | VAL  |
| 43  | 16    | 64  | LEU  |
| 43  | 16    | 65  | ILE  |
| 43  | 16    | 78  | ARG  |
| 43  | 16    | 79  | VAL  |
| 43  | 16    | 84  | VAL  |
| 43  | 16    | 89  | THR  |
| 43  | 16    | 91  | VAL  |
| 43  | 16    | 93  | VAL  |
| 43  | 16    | 98  | VAL  |
| 43  | 16    | 99  | GLU  |
| 43  | 16    | 109 | GLU  |
| 43  | 16    | 128 | LYS  |
| 43  | 16    | 131 | LYS  |
| 43  | 16    | 133 | GLU  |
| 43  | 16    | 143 | LYS  |
| 43  | 16    | 151 | LYS  |
| 43  | 16    | 152 | THR  |
| 43  | 16    | 155 | LEU  |
| 43  | 16    | 175 | LYS  |
| 44  | 17    | 22  | THR  |
| 44  | 17    | 26  | VAL  |
| 44  | 17    | 30  | ARG  |
| 44  | 17    | 40  | LYS  |
| 44  | 17    | 41  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 17    | 54  | GLU  |
| 44  | 17    | 60  | ARG  |
| 44  | 17    | 77  | VAL  |
| 44  | 17    | 83  | LEU  |
| 44  | 17    | 88  | ARG  |
| 44  | 17    | 100 | ARG  |
| 44  | 17    | 101 | LYS  |
| 44  | 17    | 110 | ARG  |
| 44  | 17    | 121 | LYS  |
| 44  | 17    | 124 | LEU  |
| 44  | 17    | 130 | ILE  |
| 44  | 17    | 156 | ILE  |
| 44  | 17    | 158 | LYS  |
| 44  | 17    | 173 | LEU  |
| 44  | 17    | 175 | LYS  |
| 44  | 17    | 178 | ILE  |
| 44  | 17    | 179 | LEU  |
| 44  | 17    | 184 | LEU  |
| 44  | 17    | 219 | LYS  |
| 44  | 17    | 228 | SER  |
| 44  | 17    | 229 | PHE  |
| 44  | 17    | 239 | LEU  |
| 45  | 18    | 41  | GLN  |
| 45  | 18    | 50  | VAL  |
| 45  | 18    | 65  | LEU  |
| 45  | 18    | 66  | SER  |
| 45  | 18    | 67  | ILE  |
| 45  | 18    | 68  | ARG  |
| 45  | 18    | 69  | LEU  |
| 45  | 18    | 71  | VAL  |
| 45  | 18    | 74  | THR  |
| 45  | 18    | 79  | GLN  |
| 45  | 18    | 81  | THR  |
| 45  | 18    | 89  | GLU  |
| 45  | 18    | 90  | THR  |
| 45  | 18    | 95  | ASN  |
| 45  | 18    | 128 | LYS  |
| 45  | 18    | 136 | LEU  |
| 45  | 18    | 145 | ASN  |
| 45  | 18    | 146 | LYS  |
| 45  | 18    | 150 | LEU  |
| 45  | 18    | 160 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | 18    | 163 | VAL  |
| 45  | 18    | 164 | VAL  |
| 45  | 18    | 166 | LEU  |
| 45  | 18    | 169 | LEU  |
| 45  | 18    | 172 | LYS  |
| 45  | 18    | 190 | VAL  |
| 45  | 18    | 192 | GLN  |
| 45  | 18    | 211 | LEU  |
| 45  | 18    | 214 | LEU  |
| 45  | 18    | 217 | THR  |
| 45  | 18    | 231 | LYS  |
| 45  | 18    | 238 | LEU  |
| 45  | 18    | 241 | LYS  |
| 45  | 18    | 248 | LYS  |
| 46  | 19    | 4   | ILE  |
| 46  | 19    | 5   | GLN  |
| 46  | 19    | 6   | THR  |
| 46  | 19    | 16  | VAL  |
| 46  | 19    | 18  | VAL  |
| 46  | 19    | 19  | SER  |
| 46  | 19    | 20  | ILE  |
| 46  | 19    | 31  | ARG  |
| 46  | 19    | 33  | THR  |
| 46  | 19    | 39  | LYS  |
| 46  | 19    | 43  | VAL  |
| 46  | 19    | 44  | THR  |
| 46  | 19    | 46  | THR  |
| 46  | 19    | 52  | LEU  |
| 46  | 19    | 55  | VAL  |
| 46  | 19    | 62  | ARG  |
| 46  | 19    | 68  | LEU  |
| 46  | 19    | 69  | ARG  |
| 46  | 19    | 70  | THR  |
| 46  | 19    | 80  | THR  |
| 46  | 19    | 82  | VAL  |
| 46  | 19    | 105 | GLU  |
| 46  | 19    | 106 | LYS  |
| 46  | 19    | 132 | VAL  |
| 46  | 19    | 133 | THR  |
| 46  | 19    | 144 | ILE  |
| 46  | 19    | 151 | VAL  |
| 46  | 19    | 157 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | l9    | 161 | LEU  |
| 46  | l9    | 162 | GLN  |
| 46  | l9    | 168 | ARG  |
| 46  | l9    | 169 | ASN  |
| 46  | l9    | 170 | LYS  |
| 46  | l9    | 173 | ARG  |
| 46  | l9    | 179 | ILE  |
| 46  | l9    | 191 | LEU  |
| 47  | m0    | 24  | ARG  |
| 47  | m0    | 26  | VAL  |
| 47  | m0    | 31  | ILE  |
| 47  | m0    | 32  | ARG  |
| 47  | m0    | 33  | ILE  |
| 47  | m0    | 36  | LEU  |
| 47  | m0    | 42  | THR  |
| 47  | m0    | 45  | GLU  |
| 47  | m0    | 48  | LEU  |
| 47  | m0    | 52  | LEU  |
| 47  | m0    | 57  | LEU  |
| 47  | m0    | 63  | GLU  |
| 47  | m0    | 69  | ARG  |
| 47  | m0    | 70  | ILE  |
| 47  | m0    | 76  | MET  |
| 47  | m0    | 77  | THR  |
| 47  | m0    | 78  | THR  |
| 47  | m0    | 82  | ARG  |
| 47  | m0    | 87  | LEU  |
| 47  | m0    | 90  | ARG  |
| 47  | m0    | 91  | VAL  |
| 47  | m0    | 99  | ILE  |
| 47  | m0    | 116 | ARG  |
| 47  | m0    | 121 | LYS  |
| 47  | m0    | 129 | VAL  |
| 47  | m0    | 130 | ASP  |
| 47  | m0    | 140 | THR  |
| 47  | m0    | 143 | SER  |
| 47  | m0    | 145 | LYS  |
| 47  | m0    | 148 | VAL  |
| 47  | m0    | 166 | ILE  |
| 47  | m0    | 167 | LEU  |
| 47  | m0    | 169 | LYS  |
| 47  | m0    | 182 | LEU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | m0    | 183 | LYS  |
| 47  | m0    | 184 | LYS  |
| 47  | m0    | 185 | ARG  |
| 47  | m0    | 197 | VAL  |
| 47  | m0    | 205 | SER  |
| 47  | m0    | 206 | LEU  |
| 47  | m0    | 211 | ARG  |
| 47  | m0    | 212 | GLU  |
| 47  | m0    | 215 | GLU  |
| 48  | m1    | 10  | ARG  |
| 48  | m1    | 12  | LEU  |
| 48  | m1    | 13  | LYS  |
| 48  | m1    | 30  | LEU  |
| 48  | m1    | 31  | THR  |
| 48  | m1    | 44  | THR  |
| 48  | m1    | 46  | VAL  |
| 48  | m1    | 54  | VAL  |
| 48  | m1    | 55  | ARG  |
| 48  | m1    | 71  | VAL  |
| 48  | m1    | 80  | LEU  |
| 48  | m1    | 85  | LYS  |
| 48  | m1    | 94  | ARG  |
| 48  | m1    | 101 | ASN  |
| 48  | m1    | 107 | ASP  |
| 48  | m1    | 112 | LEU  |
| 48  | m1    | 114 | ILE  |
| 48  | m1    | 129 | VAL  |
| 48  | m1    | 130 | VAL  |
| 48  | m1    | 133 | ARG  |
| 48  | m1    | 137 | ARG  |
| 48  | m1    | 138 | VAL  |
| 48  | m1    | 140 | ARG  |
| 48  | m1    | 142 | LYS  |
| 48  | m1    | 147 | THR  |
| 48  | m1    | 153 | LYS  |
| 48  | m1    | 159 | THR  |
| 48  | m1    | 160 | VAL  |
| 48  | m1    | 161 | SER  |
| 48  | m1    | 174 | LYS  |
| 49  | m3    | 9   | ILE  |
| 49  | m3    | 54  | LEU  |
| 49  | m3    | 55  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | m3    | 57  | VAL  |
| 49  | m3    | 58  | VAL  |
| 49  | m3    | 63  | VAL  |
| 49  | m3    | 67  | ARG  |
| 49  | m3    | 68  | LYS  |
| 49  | m3    | 69  | VAL  |
| 49  | m3    | 73  | ARG  |
| 49  | m3    | 85  | LEU  |
| 49  | m3    | 107 | GLU  |
| 49  | m3    | 114 | GLN  |
| 49  | m3    | 118 | GLU  |
| 49  | m3    | 122 | LYS  |
| 49  | m3    | 124 | ILE  |
| 49  | m3    | 128 | ARG  |
| 49  | m3    | 131 | LYS  |
| 49  | m3    | 152 | THR  |
| 49  | m3    | 164 | GLU  |
| 49  | m3    | 165 | SER  |
| 49  | m3    | 174 | ARG  |
| 49  | m3    | 184 | GLU  |
| 49  | m3    | 190 | LYS  |
| 49  | m3    | 194 | GLU  |
| 50  | m4    | 3   | THR  |
| 50  | m4    | 13  | ARG  |
| 50  | m4    | 15  | VAL  |
| 50  | m4    | 20  | VAL  |
| 50  | m4    | 27  | GLN  |
| 50  | m4    | 35  | ILE  |
| 50  | m4    | 42  | LYS  |
| 50  | m4    | 50  | LYS  |
| 50  | m4    | 53  | VAL  |
| 50  | m4    | 58  | ILE  |
| 50  | m4    | 62  | GLN  |
| 50  | m4    | 63  | VAL  |
| 50  | m4    | 64  | VAL  |
| 50  | m4    | 72  | LEU  |
| 50  | m4    | 80  | THR  |
| 50  | m4    | 82  | SER  |
| 50  | m4    | 105 | GLN  |
| 50  | m4    | 108 | ARG  |
| 50  | m4    | 113 | THR  |
| 50  | m4    | 126 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | m4    | 130 | THR  |
| 50  | m4    | 133 | LYS  |
| 50  | m4    | 135 | LEU  |
| 51  | m5    | 5   | LYS  |
| 51  | m5    | 8   | GLU  |
| 51  | m5    | 10  | LEU  |
| 51  | m5    | 12  | ARG  |
| 51  | m5    | 22  | LEU  |
| 51  | m5    | 24  | ARG  |
| 51  | m5    | 49  | ARG  |
| 51  | m5    | 61  | ILE  |
| 51  | m5    | 76  | PRO  |
| 51  | m5    | 80  | THR  |
| 51  | m5    | 83  | LYS  |
| 51  | m5    | 85  | THR  |
| 51  | m5    | 92  | LEU  |
| 51  | m5    | 96  | ARG  |
| 51  | m5    | 97  | SER  |
| 51  | m5    | 98  | LEU  |
| 51  | m5    | 105 | ARG  |
| 51  | m5    | 106 | VAL  |
| 51  | m5    | 138 | GLN  |
| 51  | m5    | 142 | ILE  |
| 51  | m5    | 153 | ASP  |
| 51  | m5    | 155 | VAL  |
| 51  | m5    | 159 | ARG  |
| 51  | m5    | 170 | LYS  |
| 51  | m5    | 176 | LYS  |
| 51  | m5    | 188 | ARG  |
| 51  | m5    | 190 | THR  |
| 51  | m5    | 194 | GLN  |
| 51  | m5    | 196 | THR  |
| 52  | m6    | 12  | LYS  |
| 52  | m6    | 16  | VAL  |
| 52  | m6    | 22  | VAL  |
| 52  | m6    | 25  | LYS  |
| 52  | m6    | 34  | VAL  |
| 52  | m6    | 41  | LEU  |
| 52  | m6    | 58  | LEU  |
| 52  | m6    | 60  | LYS  |
| 52  | m6    | 67  | THR  |
| 52  | m6    | 68  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | m6    | 74  | ARG  |
| 52  | m6    | 78  | ARG  |
| 52  | m6    | 84  | LEU  |
| 52  | m6    | 85  | ARG  |
| 52  | m6    | 89  | SER  |
| 52  | m6    | 100 | GLU  |
| 52  | m6    | 106 | GLU  |
| 52  | m6    | 108 | ILE  |
| 52  | m6    | 110 | PRO  |
| 52  | m6    | 117 | ARG  |
| 52  | m6    | 124 | LEU  |
| 52  | m6    | 126 | VAL  |
| 52  | m6    | 129 | LEU  |
| 52  | m6    | 130 | LYS  |
| 52  | m6    | 134 | LYS  |
| 52  | m6    | 152 | VAL  |
| 52  | m6    | 160 | ARG  |
| 52  | m6    | 167 | TYR  |
| 52  | m6    | 171 | LYS  |
| 52  | m6    | 172 | ARG  |
| 52  | m6    | 175 | THR  |
| 52  | m6    | 182 | ASN  |
| 52  | m6    | 184 | THR  |
| 52  | m6    | 190 | VAL  |
| 52  | m6    | 197 | LEU  |
| 53  | m7    | 9   | THR  |
| 53  | m7    | 23  | ARG  |
| 53  | m7    | 24  | VAL  |
| 53  | m7    | 31  | GLU  |
| 53  | m7    | 32  | THR  |
| 53  | m7    | 41  | LEU  |
| 53  | m7    | 49  | GLU  |
| 53  | m7    | 52  | LEU  |
| 53  | m7    | 56  | ARG  |
| 53  | m7    | 74  | LYS  |
| 53  | m7    | 78  | VAL  |
| 53  | m7    | 79  | THR  |
| 53  | m7    | 89  | LYS  |
| 53  | m7    | 94  | LEU  |
| 53  | m7    | 112 | LEU  |
| 53  | m7    | 114 | VAL  |
| 53  | m7    | 119 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | m7    | 126 | ARG  |
| 53  | m7    | 127 | ARG  |
| 53  | m7    | 128 | ARG  |
| 53  | m7    | 144 | SER  |
| 54  | m8    | 3   | ILE  |
| 54  | m8    | 7   | SER  |
| 54  | m8    | 17  | THR  |
| 54  | m8    | 24  | VAL  |
| 54  | m8    | 26  | LEU  |
| 54  | m8    | 30  | VAL  |
| 54  | m8    | 31  | LYS  |
| 54  | m8    | 32  | LEU  |
| 54  | m8    | 34  | THR  |
| 54  | m8    | 41  | ASP  |
| 54  | m8    | 46  | LYS  |
| 54  | m8    | 49  | LEU  |
| 54  | m8    | 57  | ILE  |
| 54  | m8    | 59  | ARG  |
| 54  | m8    | 63  | SER  |
| 54  | m8    | 64  | VAL  |
| 54  | m8    | 69  | ARG  |
| 54  | m8    | 80  | THR  |
| 54  | m8    | 81  | VAL  |
| 54  | m8    | 86  | THR  |
| 54  | m8    | 93  | ILE  |
| 54  | m8    | 95  | GLU  |
| 54  | m8    | 100 | THR  |
| 54  | m8    | 105 | ARG  |
| 54  | m8    | 113 | LYS  |
| 54  | m8    | 127 | LEU  |
| 54  | m8    | 135 | GLN  |
| 54  | m8    | 141 | ARG  |
| 54  | m8    | 150 | VAL  |
| 54  | m8    | 170 | ARG  |
| 54  | m8    | 180 | ARG  |
| 55  | m9    | 5   | ARG  |
| 55  | m9    | 7   | GLN  |
| 55  | m9    | 10  | LEU  |
| 55  | m9    | 17  | VAL  |
| 55  | m9    | 20  | ARG  |
| 55  | m9    | 29  | THR  |
| 55  | m9    | 36  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | m9    | 39  | ASN  |
| 55  | m9    | 43  | LYS  |
| 55  | m9    | 49  | THR  |
| 55  | m9    | 52  | LYS  |
| 55  | m9    | 55  | VAL  |
| 55  | m9    | 56  | THR  |
| 55  | m9    | 60  | LYS  |
| 55  | m9    | 63  | THR  |
| 55  | m9    | 71  | ARG  |
| 55  | m9    | 74  | ARG  |
| 55  | m9    | 76  | SER  |
| 55  | m9    | 99  | LEU  |
| 55  | m9    | 106 | LEU  |
| 55  | m9    | 117 | LYS  |
| 55  | m9    | 126 | GLU  |
| 55  | m9    | 128 | LYS  |
| 55  | m9    | 134 | HIS  |
| 55  | m9    | 138 | LEU  |
| 55  | m9    | 146 | LYS  |
| 55  | m9    | 150 | GLN  |
| 55  | m9    | 152 | GLU  |
| 55  | m9    | 153 | LYS  |
| 55  | m9    | 156 | ASN  |
| 55  | m9    | 158 | GLU  |
| 55  | m9    | 164 | LEU  |
| 55  | m9    | 170 | ARG  |
| 55  | m9    | 180 | LYS  |
| 56  | n0    | 1   | MET  |
| 56  | n0    | 13  | ARG  |
| 56  | n0    | 21  | GLU  |
| 56  | n0    | 23  | LYS  |
| 56  | n0    | 45  | LEU  |
| 56  | n0    | 51  | VAL  |
| 56  | n0    | 60  | SER  |
| 56  | n0    | 61  | ILE  |
| 56  | n0    | 63  | GLN  |
| 56  | n0    | 71  | LYS  |
| 56  | n0    | 73  | LYS  |
| 56  | n0    | 80  | ARG  |
| 56  | n0    | 87  | THR  |
| 56  | n0    | 100 | VAL  |
| 56  | n0    | 104 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | n0    | 105 | THR  |
| 56  | n0    | 106 | LEU  |
| 56  | n0    | 115 | ARG  |
| 56  | n0    | 117 | ARG  |
| 56  | n0    | 120 | SER  |
| 56  | n0    | 130 | GLU  |
| 56  | n0    | 136 | LYS  |
| 56  | n0    | 137 | ARG  |
| 56  | n0    | 138 | GLN  |
| 56  | n0    | 141 | LYS  |
| 56  | n0    | 142 | GLN  |
| 56  | n0    | 148 | LEU  |
| 56  | n0    | 149 | LYS  |
| 56  | n0    | 155 | ARG  |
| 56  | n0    | 161 | LYS  |
| 56  | n0    | 162 | THR  |
| 56  | n0    | 172 | TYR  |
| 57  | n1    | 12  | ARG  |
| 57  | n1    | 25  | VAL  |
| 57  | n1    | 26  | HIS  |
| 57  | n1    | 27  | LEU  |
| 57  | n1    | 35  | LYS  |
| 57  | n1    | 36  | VAL  |
| 57  | n1    | 68  | THR  |
| 57  | n1    | 71  | SER  |
| 57  | n1    | 78  | LYS  |
| 57  | n1    | 80  | VAL  |
| 57  | n1    | 83  | ARG  |
| 57  | n1    | 88  | ARG  |
| 57  | n1    | 89  | LEU  |
| 57  | n1    | 96  | ILE  |
| 57  | n1    | 102 | ARG  |
| 57  | n1    | 104 | GLU  |
| 57  | n1    | 122 | GLN  |
| 57  | n1    | 126 | VAL  |
| 57  | n1    | 130 | ARG  |
| 57  | n1    | 131 | GLN  |
| 57  | n1    | 135 | PRO  |
| 57  | n1    | 139 | ARG  |
| 57  | n1    | 141 | VAL  |
| 57  | n1    | 143 | THR  |
| 57  | n1    | 150 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | n1    | 160 | ILE  |
| 58  | n2    | 11  | ILE  |
| 58  | n2    | 13  | LYS  |
| 58  | n2    | 21  | SER  |
| 58  | n2    | 27  | VAL  |
| 58  | n2    | 37  | LEU  |
| 58  | n2    | 43  | VAL  |
| 58  | n2    | 54  | VAL  |
| 58  | n2    | 63  | VAL  |
| 58  | n2    | 64  | THR  |
| 58  | n2    | 66  | VAL  |
| 58  | n2    | 68  | THR  |
| 58  | n2    | 74  | LYS  |
| 58  | n2    | 90  | ARG  |
| 58  | n2    | 98  | THR  |
| 58  | n2    | 105 | LEU  |
| 59  | n3    | 13  | ILE  |
| 59  | n3    | 14  | SER  |
| 59  | n3    | 48  | ARG  |
| 59  | n3    | 73  | VAL  |
| 59  | n3    | 74  | MET  |
| 59  | n3    | 88  | ARG  |
| 59  | n3    | 91  | VAL  |
| 59  | n3    | 110 | LYS  |
| 59  | n3    | 115 | THR  |
| 60  | n4    | 1   | MET  |
| 60  | n4    | 2   | LYS  |
| 60  | n4    | 5   | ILE  |
| 60  | n4    | 26  | SER  |
| 60  | n4    | 34  | SER  |
| 60  | n4    | 39  | LEU  |
| 60  | n4    | 43  | ARG  |
| 60  | n4    | 54  | LEU  |
| 60  | n4    | 63  | ILE  |
| 60  | n4    | 96  | LEU  |
| 60  | n4    | 99  | GLU  |
| 60  | n4    | 100 | VAL  |
| 60  | n4    | 107 | GLU  |
| 60  | n4    | 119 | GLU  |
| 60  | n4    | 127 | LYS  |
| 61  | n5    | 24  | LEU  |
| 61  | n5    | 27  | ARG  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | n5    | 33  | ARG  |
| 61  | n5    | 34  | LEU  |
| 61  | n5    | 37  | THR  |
| 61  | n5    | 38  | LEU  |
| 61  | n5    | 39  | LYS  |
| 61  | n5    | 40  | LEU  |
| 61  | n5    | 45  | LYS  |
| 61  | n5    | 56  | ARG  |
| 61  | n5    | 57  | LEU  |
| 61  | n5    | 63  | ILE  |
| 61  | n5    | 64  | GLU  |
| 61  | n5    | 65  | GLN  |
| 61  | n5    | 71  | THR  |
| 61  | n5    | 74  | LYS  |
| 61  | n5    | 86  | VAL  |
| 61  | n5    | 100 | LYS  |
| 61  | n5    | 102 | LEU  |
| 61  | n5    | 106 | ASP  |
| 61  | n5    | 108 | LEU  |
| 61  | n5    | 109 | LYS  |
| 61  | n5    | 115 | ARG  |
| 61  | n5    | 125 | ARG  |
| 61  | n5    | 133 | LEU  |
| 61  | n5    | 135 | ILE  |
| 61  | n5    | 142 | ILE  |
| 62  | n6    | 4   | GLN  |
| 62  | n6    | 12  | ARG  |
| 62  | n6    | 13  | ARG  |
| 62  | n6    | 17  | LYS  |
| 62  | n6    | 37  | LYS  |
| 62  | n6    | 39  | LEU  |
| 62  | n6    | 40  | ARG  |
| 62  | n6    | 45  | ILE  |
| 62  | n6    | 50  | ILE  |
| 62  | n6    | 51  | ARG  |
| 62  | n6    | 55  | GLU  |
| 62  | n6    | 56  | VAL  |
| 62  | n6    | 57  | LEU  |
| 62  | n6    | 66  | GLN  |
| 62  | n6    | 71  | SER  |
| 62  | n6    | 76  | LEU  |
| 62  | n6    | 80  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | n6    | 83  | ASP  |
| 62  | n6    | 94  | SER  |
| 62  | n6    | 95  | VAL  |
| 62  | n6    | 97  | ILE  |
| 62  | n6    | 108 | LYS  |
| 62  | n6    | 113 | LYS  |
| 62  | n6    | 115 | ARG  |
| 62  | n6    | 120 | GLN  |
| 62  | n6    | 127 | GLU  |
| 63  | n7    | 3   | LYS  |
| 63  | n7    | 14  | VAL  |
| 63  | n7    | 17  | ARG  |
| 63  | n7    | 24  | VAL  |
| 63  | n7    | 26  | VAL  |
| 63  | n7    | 33  | SER  |
| 63  | n7    | 36  | HIS  |
| 63  | n7    | 43  | VAL  |
| 63  | n7    | 46  | ILE  |
| 63  | n7    | 52  | LYS  |
| 63  | n7    | 55  | LYS  |
| 63  | n7    | 72  | ILE  |
| 63  | n7    | 73  | LYS  |
| 63  | n7    | 75  | VAL  |
| 63  | n7    | 81  | LEU  |
| 63  | n7    | 83  | THR  |
| 63  | n7    | 86  | THR  |
| 63  | n7    | 93  | LYS  |
| 63  | n7    | 94  | SER  |
| 63  | n7    | 102 | GLU  |
| 63  | n7    | 103 | GLN  |
| 63  | n7    | 111 | LYS  |
| 63  | n7    | 121 | ARG  |
| 63  | n7    | 126 | LYS  |
| 63  | n7    | 133 | LYS  |
| 63  | n7    | 134 | LEU  |
| 63  | n7    | 135 | ARG  |
| 64  | n8    | 6   | THR  |
| 64  | n8    | 8   | THR  |
| 64  | n8    | 10  | LYS  |
| 64  | n8    | 12  | ARG  |
| 64  | n8    | 16  | SER  |
| 64  | n8    | 24  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 64  | n8    | 26  | ARG  |
| 64  | n8    | 27  | LYS  |
| 64  | n8    | 42  | ARG  |
| 64  | n8    | 47  | LYS  |
| 64  | n8    | 56  | VAL  |
| 64  | n8    | 60  | TYR  |
| 64  | n8    | 65  | GLN  |
| 64  | n8    | 70  | LYS  |
| 64  | n8    | 73  | LEU  |
| 64  | n8    | 78  | LEU  |
| 64  | n8    | 85  | ASP  |
| 64  | n8    | 91  | LEU  |
| 64  | n8    | 97  | GLU  |
| 64  | n8    | 98  | THR  |
| 64  | n8    | 115 | LYS  |
| 64  | n8    | 128 | ARG  |
| 64  | n8    | 130 | VAL  |
| 64  | n8    | 132 | LYS  |
| 64  | n8    | 133 | LEU  |
| 65  | n9    | 12  | GLN  |
| 65  | n9    | 14  | ARG  |
| 65  | n9    | 21  | ILE  |
| 65  | n9    | 22  | LYS  |
| 65  | n9    | 26  | THR  |
| 65  | n9    | 31  | SER  |
| 65  | n9    | 33  | LYS  |
| 65  | n9    | 38  | LYS  |
| 65  | n9    | 50  | THR  |
| 65  | n9    | 52  | LYS  |
| 65  | n9    | 58  | LYS  |
| 65  | n9    | 59  | LYS  |
| 66  | o0    | 8   | GLU  |
| 66  | o0    | 9   | SER  |
| 66  | o0    | 10  | ILE  |
| 66  | o0    | 18  | ILE  |
| 66  | o0    | 31  | VAL  |
| 66  | o0    | 33  | SER  |
| 66  | o0    | 34  | LEU  |
| 66  | o0    | 41  | LEU  |
| 66  | o0    | 61  | MET  |
| 66  | o0    | 76  | GLU  |
| 66  | o0    | 81  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | o0    | 86  | ARG  |
| 66  | o0    | 87  | VAL  |
| 66  | o0    | 97  | ASP  |
| 66  | o0    | 101 | LEU  |
| 66  | o0    | 103 | THR  |
| 67  | o1    | 6   | ASP  |
| 67  | o1    | 8   | VAL  |
| 67  | o1    | 13  | THR  |
| 67  | o1    | 16  | LEU  |
| 67  | o1    | 26  | LYS  |
| 67  | o1    | 31  | ARG  |
| 67  | o1    | 34  | LYS  |
| 67  | o1    | 36  | ILE  |
| 67  | o1    | 42  | LEU  |
| 67  | o1    | 44  | MET  |
| 67  | o1    | 50  | ARG  |
| 67  | o1    | 55  | LEU  |
| 67  | o1    | 61  | LYS  |
| 67  | o1    | 64  | VAL  |
| 67  | o1    | 82  | GLU  |
| 67  | o1    | 83  | GLU  |
| 67  | o1    | 89  | LEU  |
| 67  | o1    | 96  | VAL  |
| 67  | o1    | 102 | LYS  |
| 67  | o1    | 104 | LEU  |
| 67  | o1    | 106 | THR  |
| 67  | o1    | 107 | VAL  |
| 67  | o1    | 110 | GLU  |
| 68  | o2    | 4   | LEU  |
| 68  | o2    | 5   | PRO  |
| 68  | o2    | 16  | LYS  |
| 68  | o2    | 18  | LYS  |
| 68  | o2    | 19  | ARG  |
| 68  | o2    | 27  | ARG  |
| 68  | o2    | 31  | ASN  |
| 68  | o2    | 33  | ARG  |
| 68  | o2    | 34  | LYS  |
| 68  | o2    | 41  | VAL  |
| 68  | o2    | 50  | ILE  |
| 68  | o2    | 54  | LYS  |
| 68  | o2    | 73  | THR  |
| 68  | o2    | 75  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | o2    | 76  | VAL  |
| 68  | o2    | 82  | LEU  |
| 68  | o2    | 91  | THR  |
| 68  | o2    | 106 | VAL  |
| 68  | o2    | 125 | ARG  |
| 69  | o3    | 10  | LYS  |
| 69  | o3    | 20  | LYS  |
| 69  | o3    | 31  | LYS  |
| 69  | o3    | 49  | ILE  |
| 69  | o3    | 70  | LYS  |
| 69  | o3    | 81  | VAL  |
| 69  | o3    | 98  | VAL  |
| 69  | o3    | 107 | ILE  |
| 70  | o4    | 5   | VAL  |
| 70  | o4    | 16  | ARG  |
| 70  | o4    | 19  | LYS  |
| 70  | o4    | 20  | ILE  |
| 70  | o4    | 24  | LYS  |
| 70  | o4    | 29  | ILE  |
| 70  | o4    | 30  | LEU  |
| 70  | o4    | 37  | LYS  |
| 70  | o4    | 58  | ARG  |
| 70  | o4    | 64  | THR  |
| 70  | o4    | 65  | VAL  |
| 70  | o4    | 68  | THR  |
| 70  | o4    | 88  | ARG  |
| 70  | o4    | 98  | GLN  |
| 70  | o4    | 103 | LYS  |
| 70  | o4    | 104 | VAL  |
| 70  | o4    | 110 | GLU  |
| 71  | o5    | 4   | VAL  |
| 71  | o5    | 15  | GLU  |
| 71  | o5    | 20  | GLN  |
| 71  | o5    | 21  | LEU  |
| 71  | o5    | 28  | LEU  |
| 71  | o5    | 31  | LEU  |
| 71  | o5    | 38  | ARG  |
| 71  | o5    | 43  | LYS  |
| 71  | o5    | 45  | LYS  |
| 71  | o5    | 47  | VAL  |
| 71  | o5    | 48  | ARG  |
| 71  | o5    | 49  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71  | o5    | 62  | GLN  |
| 71  | o5    | 68  | GLN  |
| 71  | o5    | 69  | LEU  |
| 71  | o5    | 73  | LYS  |
| 71  | o5    | 79  | ASP  |
| 71  | o5    | 81  | ARG  |
| 71  | o5    | 84  | LYS  |
| 71  | o5    | 85  | THR  |
| 71  | o5    | 89  | ARG  |
| 71  | o5    | 90  | ARG  |
| 71  | o5    | 94  | LYS  |
| 71  | o5    | 98  | SER  |
| 71  | o5    | 100 | VAL  |
| 71  | o5    | 101 | THR  |
| 71  | o5    | 104 | GLN  |
| 71  | o5    | 119 | LYS  |
| 72  | o6    | 3   | VAL  |
| 72  | o6    | 4   | LYS  |
| 72  | o6    | 7   | ILE  |
| 72  | o6    | 9   | ILE  |
| 72  | o6    | 11  | LEU  |
| 72  | o6    | 17  | VAL  |
| 72  | o6    | 21  | THR  |
| 72  | o6    | 25  | LYS  |
| 72  | o6    | 26  | ILE  |
| 72  | o6    | 29  | LYS  |
| 72  | o6    | 34  | SER  |
| 72  | o6    | 36  | ARG  |
| 72  | o6    | 37  | THR  |
| 72  | o6    | 38  | LYS  |
| 72  | o6    | 43  | LEU  |
| 72  | o6    | 45  | ARG  |
| 72  | o6    | 57  | LEU  |
| 72  | o6    | 58  | ILE  |
| 72  | o6    | 60  | LEU  |
| 72  | o6    | 64  | SER  |
| 72  | o6    | 74  | LYS  |
| 72  | o6    | 75  | LYS  |
| 72  | o6    | 76  | ARG  |
| 72  | o6    | 81  | THR  |
| 72  | o6    | 88  | GLU  |
| 72  | o6    | 94  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | o6    | 98  | ARG  |
| 73  | o7    | 17  | THR  |
| 73  | o7    | 24  | ARG  |
| 73  | o7    | 25  | ARG  |
| 73  | o7    | 33  | THR  |
| 73  | o7    | 36  | SER  |
| 73  | o7    | 44  | THR  |
| 73  | o7    | 55  | ARG  |
| 73  | o7    | 58  | THR  |
| 73  | o7    | 67  | LEU  |
| 73  | o7    | 68  | LYS  |
| 73  | o7    | 80  | THR  |
| 74  | o8    | 5   | ILE  |
| 74  | o8    | 12  | LEU  |
| 74  | o8    | 17  | ARG  |
| 74  | o8    | 41  | THR  |
| 74  | o8    | 53  | THR  |
| 74  | o8    | 61  | LYS  |
| 74  | o8    | 64  | LYS  |
| 74  | o8    | 65  | LEU  |
| 74  | o8    | 68  | SER  |
| 74  | o8    | 72  | THR  |
| 75  | o9    | 4   | GLN  |
| 75  | o9    | 15  | LYS  |
| 75  | o9    | 17  | LYS  |
| 75  | o9    | 19  | GLN  |
| 75  | o9    | 21  | ARG  |
| 75  | o9    | 23  | LEU  |
| 75  | o9    | 27  | ILE  |
| 75  | o9    | 29  | LEU  |
| 75  | o9    | 30  | ARG  |
| 75  | o9    | 45  | ARG  |
| 75  | o9    | 47  | THR  |
| 75  | o9    | 48  | LYS  |
| 75  | o9    | 51  | ILE  |
| 76  | q0    | 77  | ILE  |
| 76  | q0    | 78  | ILE  |
| 76  | q0    | 85  | LEU  |
| 76  | q0    | 88  | LYS  |
| 76  | q0    | 93  | LYS  |
| 76  | q0    | 112 | LYS  |
| 76  | q0    | 113 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 76  | q0    | 114 | LYS  |
| 76  | q0    | 127 | LEU  |
| 77  | q1    | 2   | ARG  |
| 77  | q1    | 6   | ARG  |
| 77  | q1    | 9   | ARG  |
| 77  | q1    | 10  | THR  |
| 77  | q1    | 13  | LEU  |
| 77  | q1    | 14  | LYS  |
| 77  | q1    | 16  | LYS  |
| 77  | q1    | 21  | ARG  |
| 77  | q1    | 23  | ARG  |
| 77  | q1    | 24  | SER  |
| 78  | q2    | 2   | VAL  |
| 78  | q2    | 7   | THR  |
| 78  | q2    | 8   | ARG  |
| 78  | q2    | 15  | LYS  |
| 78  | q2    | 16  | THR  |
| 78  | q2    | 17  | CYS  |
| 78  | q2    | 46  | LYS  |
| 78  | q2    | 48  | SER  |
| 78  | q2    | 63  | LYS  |
| 78  | q2    | 71  | ARG  |
| 78  | q2    | 78  | LYS  |
| 78  | q2    | 79  | THR  |
| 78  | q2    | 83  | LEU  |
| 78  | q2    | 84  | THR  |
| 78  | q2    | 85  | LEU  |
| 78  | q2    | 93  | LEU  |
| 78  | q2    | 100 | LYS  |
| 78  | q2    | 104 | LEU  |
| 78  | q2    | 105 | GLN  |
| 79  | q3    | 3   | LYS  |
| 79  | q3    | 5   | THR  |
| 79  | q3    | 10  | ILE  |
| 79  | q3    | 16  | VAL  |
| 79  | q3    | 22  | LEU  |
| 79  | q3    | 33  | GLN  |
| 79  | q3    | 42  | CYS  |
| 79  | q3    | 48  | LYS  |
| 79  | q3    | 49  | ARG  |
| 79  | q3    | 54  | ILE  |
| 79  | q3    | 56  | THR  |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 79         | q3           | 62         | LYS         |
| 79         | q3           | 78         | THR         |
| 79         | q3           | 90         | VAL         |
| 82         | p0           | 4          | ILE         |
| 82         | p0           | 5          | ARG         |
| 82         | p0           | 10         | GLU         |
| 82         | p0           | 15         | LEU         |
| 82         | p0           | 17         | GLU         |
| 82         | p0           | 25         | LEU         |
| 82         | p0           | 39         | HIS         |
| 82         | p0           | 42         | ARG         |
| 82         | p0           | 43         | LYS         |
| 82         | p0           | 44         | GLU         |
| 82         | p0           | 52         | LEU         |
| 82         | p0           | 55         | LYS         |
| 82         | p0           | 69         | ASP         |
| 82         | p0           | 70         | LEU         |
| 82         | p0           | 72         | ASP         |
| 82         | p0           | 76         | LEU         |
| 82         | p0           | 81         | LYS         |
| 82         | p0           | 91         | GLU         |
| 82         | p0           | 93         | LEU         |
| 82         | p0           | 94         | THR         |
| 82         | p0           | 96         | ILE         |
| 82         | p0           | 97         | LYS         |
| 82         | p0           | 103        | ASN         |
| 82         | p0           | 104        | ARG         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | S0           | 163        | ASN         |
| 2          | S0           | 168        | HIS         |
| 3          | S1           | 79         | HIS         |
| 5          | S3           | 101        | GLN         |
| 5          | S3           | 159        | HIS         |
| 6          | S4           | 17         | HIS         |
| 6          | S4           | 50         | ASN         |
| 6          | S4           | 67         | GLN         |
| 6          | S4           | 98         | ASN         |
| 6          | S4           | 142        | HIS         |
| 6          | S4           | 188        | ASN         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | S4    | 197 | HIS  |
| 7   | S5    | 35  | GLN  |
| 7   | S5    | 103 | ASN  |
| 7   | S5    | 139 | ASN  |
| 8   | S6    | 13  | GLN  |
| 8   | S6    | 119 | GLN  |
| 9   | S7    | 71  | HIS  |
| 9   | S7    | 174 | ASN  |
| 9   | S7    | 180 | GLN  |
| 10  | S8    | 88  | ASN  |
| 10  | S8    | 94  | ASN  |
| 11  | S9    | 110 | GLN  |
| 11  | S9    | 112 | GLN  |
| 12  | C0    | 58  | GLN  |
| 13  | C1    | 21  | ASN  |
| 19  | C7    | 101 | ASN  |
| 20  | C8    | 6   | GLN  |
| 20  | C8    | 104 | ASN  |
| 21  | C9    | 23  | GLN  |
| 22  | D0    | 40  | ASN  |
| 23  | D1    | 7   | GLN  |
| 23  | D1    | 74  | GLN  |
| 24  | D2    | 39  | GLN  |
| 24  | D2    | 70  | ASN  |
| 26  | D4    | 63  | GLN  |
| 27  | D5    | 44  | GLN  |
| 27  | D5    | 95  | HIS  |
| 28  | D6    | 72  | HIS  |
| 29  | D7    | 9   | HIS  |
| 29  | D7    | 51  | GLN  |
| 31  | D9    | 48  | ASN  |
| 33  | E1    | 135 | HIS  |
| 34  | SR    | 17  | ASN  |
| 34  | SR    | 174 | ASN  |
| 34  | SR    | 187 | GLN  |
| 34  | SR    | 268 | GLN  |
| 35  | SM    | 70  | ASN  |
| 39  | L2    | 47  | GLN  |
| 39  | L2    | 83  | HIS  |
| 39  | L2    | 115 | ASN  |
| 39  | L2    | 209 | HIS  |
| 39  | L2    | 250 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | L3    | 224 | HIS  |
| 40  | L3    | 231 | HIS  |
| 41  | L4    | 116 | ASN  |
| 42  | L5    | 40  | HIS  |
| 42  | L5    | 57  | ASN  |
| 43  | L6    | 61  | ASN  |
| 44  | L7    | 244 | ASN  |
| 45  | L8    | 232 | HIS  |
| 46  | L9    | 5   | GLN  |
| 47  | M0    | 59  | GLN  |
| 47  | M0    | 100 | ASN  |
| 47  | M0    | 163 | GLN  |
| 48  | M1    | 47  | GLN  |
| 48  | M1    | 68  | HIS  |
| 48  | M1    | 95  | ASN  |
| 49  | M3    | 19  | GLN  |
| 50  | M4    | 59  | ASN  |
| 52  | M6    | 122 | GLN  |
| 53  | M7    | 133 | HIS  |
| 53  | M7    | 137 | ASN  |
| 53  | M7    | 172 | GLN  |
| 54  | M8    | 45  | ASN  |
| 54  | M8    | 73  | GLN  |
| 54  | M8    | 126 | GLN  |
| 55  | M9    | 141 | HIS  |
| 55  | M9    | 144 | GLN  |
| 57  | N1    | 26  | HIS  |
| 58  | N2    | 88  | GLN  |
| 59  | N3    | 81  | GLN  |
| 59  | N3    | 98  | ASN  |
| 60  | N4    | 42  | GLN  |
| 63  | N7    | 106 | GLN  |
| 63  | N7    | 122 | HIS  |
| 64  | N8    | 11  | HIS  |
| 64  | N8    | 28  | HIS  |
| 65  | N9    | 43  | HIS  |
| 66  | O0    | 11  | ASN  |
| 67  | O1    | 21  | HIS  |
| 68  | O2    | 20  | HIS  |
| 68  | O2    | 49  | ASN  |
| 69  | O3    | 42  | GLN  |
| 71  | O5    | 62  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71  | O5    | 68  | GLN  |
| 71  | O5    | 99  | GLN  |
| 72  | O6    | 63  | ASN  |
| 73  | O7    | 12  | HIS  |
| 73  | O7    | 79  | GLN  |
| 79  | Q3    | 32  | GLN  |
| 79  | Q3    | 33  | GLN  |
| 2   | s0    | 33  | GLN  |
| 2   | s0    | 46  | HIS  |
| 2   | s0    | 69  | ASN  |
| 2   | s0    | 140 | ASN  |
| 3   | s1    | 146 | GLN  |
| 3   | s1    | 209 | ASN  |
| 3   | s1    | 211 | HIS  |
| 3   | s1    | 220 | GLN  |
| 4   | s2    | 59  | HIS  |
| 4   | s2    | 228 | ASN  |
| 6   | s4    | 216 | ASN  |
| 8   | s6    | 197 | ASN  |
| 9   | s7    | 5   | GLN  |
| 10  | s8    | 138 | ASN  |
| 11  | s9    | 110 | GLN  |
| 12  | c0    | 28  | ASN  |
| 12  | c0    | 32  | HIS  |
| 12  | c0    | 58  | GLN  |
| 13  | c1    | 92  | HIS  |
| 14  | c2    | 38  | HIS  |
| 15  | c3    | 49  | GLN  |
| 15  | c3    | 62  | GLN  |
| 18  | c6    | 21  | HIS  |
| 18  | c6    | 103 | ASN  |
| 19  | c7    | 101 | ASN  |
| 20  | c8    | 25  | ASN  |
| 20  | c8    | 127 | HIS  |
| 22  | d0    | 16  | GLN  |
| 22  | d0    | 49  | ASN  |
| 24  | d2    | 42  | GLN  |
| 24  | d2    | 56  | HIS  |
| 24  | d2    | 70  | ASN  |
| 24  | d2    | 98  | GLN  |
| 26  | d4    | 22  | GLN  |
| 26  | d4    | 77  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | d4    | 106 | GLN  |
| 29  | d7    | 26  | GLN  |
| 30  | d8    | 51  | ASN  |
| 80  | e0    | 46  | ASN  |
| 33  | e1    | 93  | HIS  |
| 34  | sR    | 29  | GLN  |
| 34  | sR    | 101 | GLN  |
| 34  | sR    | 153 | GLN  |
| 34  | sR    | 184 | ASN  |
| 39  | l2    | 97  | ASN  |
| 39  | l2    | 194 | ASN  |
| 39  | l2    | 205 | ASN  |
| 40  | l3    | 182 | GLN  |
| 40  | l3    | 224 | HIS  |
| 40  | l3    | 259 | HIS  |
| 41  | l4    | 160 | GLN  |
| 41  | l4    | 201 | GLN  |
| 41  | l4    | 229 | ASN  |
| 42  | l5    | 111 | GLN  |
| 42  | l5    | 264 | GLN  |
| 44  | l7    | 112 | ASN  |
| 45  | l8    | 33  | ASN  |
| 45  | l8    | 38  | GLN  |
| 45  | l8    | 192 | GLN  |
| 45  | l8    | 243 | GLN  |
| 46  | l9    | 96  | HIS  |
| 47  | m0    | 55  | ASN  |
| 47  | m0    | 59  | GLN  |
| 47  | m0    | 163 | GLN  |
| 50  | m4    | 56  | GLN  |
| 51  | m5    | 123 | GLN  |
| 51  | m5    | 156 | HIS  |
| 53  | m7    | 92  | GLN  |
| 53  | m7    | 125 | GLN  |
| 54  | m8    | 73  | GLN  |
| 56  | n0    | 108 | GLN  |
| 56  | n0    | 138 | GLN  |
| 57  | n1    | 131 | GLN  |
| 60  | n4    | 42  | GLN  |
| 60  | n4    | 59  | HIS  |
| 61  | n5    | 85  | GLN  |
| 61  | n5    | 111 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | n6    | 81  | GLN  |
| 62  | n6    | 120 | GLN  |
| 63  | n7    | 36  | HIS  |
| 64  | n8    | 28  | HIS  |
| 65  | n9    | 19  | ASN  |
| 70  | o4    | 33  | GLN  |
| 70  | o4    | 69  | HIS  |
| 70  | o4    | 98  | GLN  |
| 71  | o5    | 34  | GLN  |
| 75  | o9    | 11  | GLN  |
| 75  | o9    | 19  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1   | 2     | 1747/1800 (97%)   | 453 (25%)         | 63 (3%)         |
| 1   | 6     | 1794/1800 (99%)   | 436 (24%)         | 59 (3%)         |
| 36  | 1     | 3145/3396 (92%)   | 624 (19%)         | 99 (3%)         |
| 36  | 5     | 3145/3396 (92%)   | 632 (20%)         | 101 (3%)        |
| 37  | 3     | 120/121 (99%)     | 17 (14%)          | 2 (1%)          |
| 37  | 7     | 120/121 (99%)     | 15 (12%)          | 1 (0%)          |
| 38  | 4     | 157/158 (99%)     | 36 (22%)          | 3 (1%)          |
| 38  | 8     | 157/158 (99%)     | 37 (23%)          | 2 (1%)          |
| All | All   | 10385/10950 (94%) | 2250 (21%)        | 330 (3%)        |

All (2250) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | A    |
| 1   | 2     | 4   | C    |
| 1   | 2     | 17  | C    |
| 1   | 2     | 25  | C    |
| 1   | 2     | 26  | A    |
| 1   | 2     | 27  | U    |
| 1   | 2     | 34  | G    |
| 1   | 2     | 45  | U    |
| 1   | 2     | 46  | A    |
| 1   | 2     | 47  | A    |
| 1   | 2     | 57  | G    |
| 1   | 2     | 60  | U    |
| 1   | 2     | 67  | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 68  | A    |
| 1   | 2     | 69  | G    |
| 1   | 2     | 72  | A    |
| 1   | 2     | 73  | U    |
| 1   | 2     | 74  | U    |
| 1   | 2     | 75  | U    |
| 1   | 2     | 100 | A    |
| 1   | 2     | 103 | A    |
| 1   | 2     | 104 | A    |
| 1   | 2     | 114 | C    |
| 1   | 2     | 130 | C    |
| 1   | 2     | 131 | C    |
| 1   | 2     | 132 | U    |
| 1   | 2     | 133 | U    |
| 1   | 2     | 134 | U    |
| 1   | 2     | 135 | A    |
| 1   | 2     | 136 | C    |
| 1   | 2     | 137 | U    |
| 1   | 2     | 140 | A    |
| 1   | 2     | 141 | U    |
| 1   | 2     | 144 | U    |
| 1   | 2     | 145 | A    |
| 1   | 2     | 146 | U    |
| 1   | 2     | 158 | U    |
| 1   | 2     | 159 | U    |
| 1   | 2     | 175 | G    |
| 1   | 2     | 178 | U    |
| 1   | 2     | 179 | A    |
| 1   | 2     | 185 | U    |
| 1   | 2     | 186 | C    |
| 1   | 2     | 187 | G    |
| 1   | 2     | 190 | C    |
| 1   | 2     | 191 | C    |
| 1   | 2     | 192 | U    |
| 1   | 2     | 193 | U    |
| 1   | 2     | 194 | U    |
| 1   | 2     | 195 | G    |
| 1   | 2     | 196 | G    |
| 1   | 2     | 197 | A    |
| 1   | 2     | 198 | A    |
| 1   | 2     | 200 | A    |
| 1   | 2     | 215 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 217 | A    |
| 1   | 2     | 218 | A    |
| 1   | 2     | 219 | A    |
| 1   | 2     | 226 | A    |
| 1   | 2     | 227 | U    |
| 1   | 2     | 228 | G    |
| 1   | 2     | 229 | U    |
| 1   | 2     | 231 | U    |
| 1   | 2     | 233 | C    |
| 1   | 2     | 234 | G    |
| 1   | 2     | 235 | G    |
| 1   | 2     | 238 | U    |
| 1   | 2     | 239 | C    |
| 1   | 2     | 240 | U    |
| 1   | 2     | 241 | U    |
| 1   | 2     | 250 | C    |
| 1   | 2     | 251 | A    |
| 1   | 2     | 260 | U    |
| 1   | 2     | 261 | U    |
| 1   | 2     | 265 | A    |
| 1   | 2     | 266 | A    |
| 1   | 2     | 271 | A    |
| 1   | 2     | 272 | U    |
| 1   | 2     | 274 | G    |
| 1   | 2     | 275 | C    |
| 1   | 2     | 277 | U    |
| 1   | 2     | 278 | U    |
| 1   | 2     | 279 | G    |
| 1   | 2     | 280 | U    |
| 1   | 2     | 281 | G    |
| 1   | 2     | 288 | A    |
| 1   | 2     | 290 | G    |
| 1   | 2     | 299 | A    |
| 1   | 2     | 309 | C    |
| 1   | 2     | 314 | C    |
| 1   | 2     | 316 | A    |
| 1   | 2     | 319 | U    |
| 1   | 2     | 320 | U    |
| 1   | 2     | 321 | C    |
| 1   | 2     | 322 | G    |
| 1   | 2     | 337 | G    |
| 1   | 2     | 338 | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 352 | A    |
| 1   | 2     | 359 | A    |
| 1   | 2     | 360 | A    |
| 1   | 2     | 361 | C    |
| 1   | 2     | 390 | G    |
| 1   | 2     | 400 | A    |
| 1   | 2     | 401 | A    |
| 1   | 2     | 402 | C    |
| 1   | 2     | 404 | G    |
| 1   | 2     | 416 | A    |
| 1   | 2     | 417 | A    |
| 1   | 2     | 418 | G    |
| 1   | 2     | 424 | C    |
| 1   | 2     | 425 | A    |
| 1   | 2     | 426 | G    |
| 1   | 2     | 428 | A    |
| 1   | 2     | 434 | G    |
| 1   | 2     | 439 | U    |
| 1   | 2     | 444 | C    |
| 1   | 2     | 446 | A    |
| 1   | 2     | 448 | C    |
| 1   | 2     | 460 | A    |
| 1   | 2     | 470 | A    |
| 1   | 2     | 477 | A    |
| 1   | 2     | 480 | G    |
| 1   | 2     | 484 | C    |
| 1   | 2     | 485 | A    |
| 1   | 2     | 486 | G    |
| 1   | 2     | 488 | G    |
| 1   | 2     | 493 | U    |
| 1   | 2     | 494 | U    |
| 1   | 2     | 495 | C    |
| 1   | 2     | 496 | G    |
| 1   | 2     | 497 | G    |
| 1   | 2     | 498 | G    |
| 1   | 2     | 499 | U    |
| 1   | 2     | 500 | C    |
| 1   | 2     | 502 | U    |
| 1   | 2     | 504 | U    |
| 1   | 2     | 505 | A    |
| 1   | 2     | 506 | A    |
| 1   | 2     | 507 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 508 | U    |
| 1   | 2     | 510 | G    |
| 1   | 2     | 511 | A    |
| 1   | 2     | 512 | A    |
| 1   | 2     | 513 | U    |
| 1   | 2     | 515 | A    |
| 1   | 2     | 516 | G    |
| 1   | 2     | 527 | A    |
| 1   | 2     | 528 | U    |
| 1   | 2     | 532 | U    |
| 1   | 2     | 536 | C    |
| 1   | 2     | 538 | A    |
| 1   | 2     | 539 | G    |
| 1   | 2     | 540 | G    |
| 1   | 2     | 541 | A    |
| 1   | 2     | 542 | A    |
| 1   | 2     | 543 | C    |
| 1   | 2     | 544 | A    |
| 1   | 2     | 548 | G    |
| 1   | 2     | 555 | A    |
| 1   | 2     | 557 | G    |
| 1   | 2     | 558 | U    |
| 1   | 2     | 559 | C    |
| 1   | 2     | 565 | C    |
| 1   | 2     | 570 | A    |
| 1   | 2     | 578 | U    |
| 1   | 2     | 579 | A    |
| 1   | 2     | 580 | A    |
| 1   | 2     | 582 | U    |
| 1   | 2     | 585 | A    |
| 1   | 2     | 594 | A    |
| 1   | 2     | 595 | G    |
| 1   | 2     | 609 | U    |
| 1   | 2     | 611 | U    |
| 1   | 2     | 619 | A    |
| 1   | 2     | 620 | A    |
| 1   | 2     | 622 | A    |
| 1   | 2     | 623 | A    |
| 1   | 2     | 624 | G    |
| 1   | 2     | 639 | U    |
| 1   | 2     | 640 | U    |
| 1   | 2     | 645 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 650 | U    |
| 1   | 2     | 653 | C    |
| 1   | 2     | 654 | C    |
| 1   | 2     | 655 | G    |
| 1   | 2     | 656 | G    |
| 1   | 2     | 657 | U    |
| 1   | 2     | 658 | C    |
| 1   | 2     | 677 | G    |
| 1   | 2     | 679 | U    |
| 1   | 2     | 680 | U    |
| 1   | 2     | 682 | C    |
| 1   | 2     | 684 | A    |
| 1   | 2     | 685 | A    |
| 1   | 2     | 686 | C    |
| 1   | 2     | 693 | U    |
| 1   | 2     | 694 | U    |
| 1   | 2     | 696 | C    |
| 1   | 2     | 697 | C    |
| 1   | 2     | 700 | C    |
| 1   | 2     | 701 | U    |
| 1   | 2     | 702 | G    |
| 1   | 2     | 703 | G    |
| 1   | 2     | 704 | C    |
| 1   | 2     | 705 | U    |
| 1   | 2     | 707 | A    |
| 1   | 2     | 709 | C    |
| 1   | 2     | 710 | U    |
| 1   | 2     | 712 | G    |
| 1   | 2     | 713 | A    |
| 1   | 2     | 714 | G    |
| 1   | 2     | 717 | C    |
| 1   | 2     | 718 | U    |
| 1   | 2     | 719 | U    |
| 1   | 2     | 721 | U    |
| 1   | 2     | 722 | G    |
| 1   | 2     | 723 | G    |
| 1   | 2     | 725 | U    |
| 1   | 2     | 727 | U    |
| 1   | 2     | 728 | U    |
| 1   | 2     | 730 | G    |
| 1   | 2     | 731 | C    |
| 1   | 2     | 732 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 733 | A    |
| 1   | 2     | 734 | A    |
| 1   | 2     | 735 | C    |
| 1   | 2     | 736 | C    |
| 1   | 2     | 737 | A    |
| 1   | 2     | 738 | G    |
| 1   | 2     | 742 | U    |
| 1   | 2     | 754 | A    |
| 1   | 2     | 755 | A    |
| 1   | 2     | 756 | A    |
| 1   | 2     | 758 | U    |
| 1   | 2     | 765 | G    |
| 1   | 2     | 766 | U    |
| 1   | 2     | 774 | A    |
| 1   | 2     | 775 | G    |
| 1   | 2     | 778 | G    |
| 1   | 2     | 779 | U    |
| 1   | 2     | 780 | A    |
| 1   | 2     | 781 | U    |
| 1   | 2     | 782 | U    |
| 1   | 2     | 783 | G    |
| 1   | 2     | 784 | C    |
| 1   | 2     | 789 | A    |
| 1   | 2     | 794 | U    |
| 1   | 2     | 795 | U    |
| 1   | 2     | 811 | A    |
| 1   | 2     | 812 | A    |
| 1   | 2     | 815 | G    |
| 1   | 2     | 816 | G    |
| 1   | 2     | 818 | C    |
| 1   | 2     | 819 | G    |
| 1   | 2     | 820 | U    |
| 1   | 2     | 821 | U    |
| 1   | 2     | 822 | U    |
| 1   | 2     | 823 | G    |
| 1   | 2     | 829 | A    |
| 1   | 2     | 830 | U    |
| 1   | 2     | 831 | U    |
| 1   | 2     | 833 | U    |
| 1   | 2     | 837 | G    |
| 1   | 2     | 840 | U    |
| 1   | 2     | 846 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 856  | A    |
| 1   | 2     | 860  | U    |
| 1   | 2     | 862  | A    |
| 1   | 2     | 863  | A    |
| 1   | 2     | 864  | U    |
| 1   | 2     | 876  | G    |
| 1   | 2     | 886  | U    |
| 1   | 2     | 898  | A    |
| 1   | 2     | 912  | U    |
| 1   | 2     | 913  | G    |
| 1   | 2     | 914  | G    |
| 1   | 2     | 915  | A    |
| 1   | 2     | 916  | U    |
| 1   | 2     | 933  | A    |
| 1   | 2     | 935  | U    |
| 1   | 2     | 942  | G    |
| 1   | 2     | 959  | U    |
| 1   | 2     | 960  | U    |
| 1   | 2     | 961  | U    |
| 1   | 2     | 966  | A    |
| 1   | 2     | 974  | A    |
| 1   | 2     | 992  | A    |
| 1   | 2     | 993  | A    |
| 1   | 2     | 995  | A    |
| 1   | 2     | 997  | G    |
| 1   | 2     | 1003 | A    |
| 1   | 2     | 1004 | U    |
| 1   | 2     | 1005 | A    |
| 1   | 2     | 1020 | A    |
| 1   | 2     | 1021 | C    |
| 1   | 2     | 1026 | A    |
| 1   | 2     | 1028 | C    |
| 1   | 2     | 1031 | U    |
| 1   | 2     | 1039 | A    |
| 1   | 2     | 1040 | G    |
| 1   | 2     | 1051 | G    |
| 1   | 2     | 1052 | U    |
| 1   | 2     | 1053 | G    |
| 1   | 2     | 1058 | U    |
| 1   | 2     | 1059 | U    |
| 1   | 2     | 1060 | U    |
| 1   | 2     | 1061 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1074 | G    |
| 1   | 2     | 1079 | U    |
| 1   | 2     | 1080 | U    |
| 1   | 2     | 1082 | C    |
| 1   | 2     | 1091 | A    |
| 1   | 2     | 1092 | A    |
| 1   | 2     | 1096 | C    |
| 1   | 2     | 1097 | U    |
| 1   | 2     | 1100 | G    |
| 1   | 2     | 1111 | G    |
| 1   | 2     | 1138 | A    |
| 1   | 2     | 1139 | A    |
| 1   | 2     | 1146 | G    |
| 1   | 2     | 1151 | A    |
| 1   | 2     | 1155 | G    |
| 1   | 2     | 1157 | A    |
| 1   | 2     | 1158 | C    |
| 1   | 2     | 1160 | A    |
| 1   | 2     | 1161 | C    |
| 1   | 2     | 1167 | G    |
| 1   | 2     | 1176 | G    |
| 1   | 2     | 1185 | U    |
| 1   | 2     | 1191 | U    |
| 1   | 2     | 1194 | A    |
| 1   | 2     | 1196 | A    |
| 1   | 2     | 1197 | C    |
| 1   | 2     | 1199 | G    |
| 1   | 2     | 1200 | G    |
| 1   | 2     | 1202 | A    |
| 1   | 2     | 1203 | A    |
| 1   | 2     | 1207 | C    |
| 1   | 2     | 1208 | A    |
| 1   | 2     | 1217 | A    |
| 1   | 2     | 1218 | G    |
| 1   | 2     | 1219 | A    |
| 1   | 2     | 1226 | A    |
| 1   | 2     | 1227 | A    |
| 1   | 2     | 1228 | G    |
| 1   | 2     | 1229 | G    |
| 1   | 2     | 1235 | C    |
| 1   | 2     | 1241 | G    |
| 1   | 2     | 1242 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1244 | A    |
| 1   | 2     | 1245 | G    |
| 1   | 2     | 1250 | U    |
| 1   | 2     | 1251 | U    |
| 1   | 2     | 1257 | U    |
| 1   | 2     | 1258 | U    |
| 1   | 2     | 1260 | U    |
| 1   | 2     | 1286 | U    |
| 1   | 2     | 1310 | U    |
| 1   | 2     | 1314 | U    |
| 1   | 2     | 1315 | U    |
| 1   | 2     | 1320 | U    |
| 1   | 2     | 1321 | A    |
| 1   | 2     | 1337 | A    |
| 1   | 2     | 1339 | C    |
| 1   | 2     | 1340 | U    |
| 1   | 2     | 1341 | A    |
| 1   | 2     | 1344 | A    |
| 1   | 2     | 1345 | A    |
| 1   | 2     | 1354 | G    |
| 1   | 2     | 1361 | U    |
| 1   | 2     | 1362 | U    |
| 1   | 2     | 1363 | U    |
| 1   | 2     | 1364 | G    |
| 1   | 2     | 1370 | U    |
| 1   | 2     | 1371 | A    |
| 1   | 2     | 1390 | U    |
| 1   | 2     | 1398 | U    |
| 1   | 2     | 1399 | C    |
| 1   | 2     | 1412 | G    |
| 1   | 2     | 1413 | U    |
| 1   | 2     | 1414 | U    |
| 1   | 2     | 1415 | U    |
| 1   | 2     | 1427 | A    |
| 1   | 2     | 1428 | G    |
| 1   | 2     | 1431 | C    |
| 1   | 2     | 1446 | A    |
| 1   | 2     | 1448 | G    |
| 1   | 2     | 1457 | C    |
| 1   | 2     | 1458 | G    |
| 1   | 2     | 1459 | C    |
| 1   | 2     | 1462 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1471 | A    |
| 1   | 2     | 1473 | U    |
| 1   | 2     | 1474 | G    |
| 1   | 2     | 1477 | G    |
| 1   | 2     | 1478 | G    |
| 1   | 2     | 1482 | C    |
| 1   | 2     | 1486 | G    |
| 1   | 2     | 1489 | U    |
| 1   | 2     | 1490 | C    |
| 1   | 2     | 1491 | U    |
| 1   | 2     | 1492 | A    |
| 1   | 2     | 1493 | A    |
| 1   | 2     | 1499 | G    |
| 1   | 2     | 1506 | G    |
| 1   | 2     | 1514 | U    |
| 1   | 2     | 1515 | A    |
| 1   | 2     | 1516 | A    |
| 1   | 2     | 1521 | G    |
| 1   | 2     | 1523 | G    |
| 1   | 2     | 1524 | A    |
| 1   | 2     | 1535 | U    |
| 1   | 2     | 1536 | G    |
| 1   | 2     | 1537 | C    |
| 1   | 2     | 1538 | U    |
| 1   | 2     | 1540 | G    |
| 1   | 2     | 1557 | U    |
| 1   | 2     | 1559 | A    |
| 1   | 2     | 1568 | C    |
| 1   | 2     | 1569 | A    |
| 1   | 2     | 1572 | G    |
| 1   | 2     | 1573 | A    |
| 1   | 2     | 1574 | G    |
| 1   | 2     | 1584 | G    |
| 1   | 2     | 1590 | G    |
| 1   | 2     | 1601 | G    |
| 1   | 2     | 1616 | G    |
| 1   | 2     | 1631 | A    |
| 1   | 2     | 1657 | U    |
| 1   | 2     | 1658 | G    |
| 1   | 2     | 1663 | G    |
| 1   | 2     | 1681 | A    |
| 1   | 2     | 1682 | U    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1683 | C    |
| 1   | 2     | 1684 | U    |
| 1   | 2     | 1731 | A    |
| 1   | 2     | 1751 | C    |
| 1   | 2     | 1756 | A    |
| 1   | 2     | 1759 | C    |
| 1   | 2     | 1760 | G    |
| 1   | 2     | 1761 | U    |
| 1   | 2     | 1762 | A    |
| 1   | 2     | 1766 | A    |
| 1   | 2     | 1769 | U    |
| 1   | 2     | 1770 | U    |
| 1   | 2     | 1780 | G    |
| 1   | 2     | 1782 | A    |
| 1   | 2     | 1783 | C    |
| 1   | 2     | 1792 | G    |
| 1   | 2     | 1793 | G    |
| 1   | 2     | 1794 | A    |
| 1   | 2     | 1795 | U    |
| 1   | 2     | 1796 | C    |
| 36  | 1     | 13   | A    |
| 36  | 1     | 14   | U    |
| 36  | 1     | 18   | G    |
| 36  | 1     | 26   | A    |
| 36  | 1     | 40   | A    |
| 36  | 1     | 43   | A    |
| 36  | 1     | 44   | U    |
| 36  | 1     | 49   | A    |
| 36  | 1     | 59   | G    |
| 36  | 1     | 60   | A    |
| 36  | 1     | 65   | A    |
| 36  | 1     | 66   | A    |
| 36  | 1     | 75   | G    |
| 36  | 1     | 77   | A    |
| 36  | 1     | 92   | G    |
| 36  | 1     | 99   | A    |
| 36  | 1     | 100  | A    |
| 36  | 1     | 109  | A    |
| 36  | 1     | 110  | G    |
| 36  | 1     | 113  | C    |
| 36  | 1     | 121  | A    |
| 36  | 1     | 122  | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 1     | 133 | U    |
| 36  | 1     | 135 | C    |
| 36  | 1     | 136 | G    |
| 36  | 1     | 142 | C    |
| 36  | 1     | 156 | G    |
| 36  | 1     | 157 | A    |
| 36  | 1     | 163 | C    |
| 36  | 1     | 166 | C    |
| 36  | 1     | 169 | U    |
| 36  | 1     | 170 | G    |
| 36  | 1     | 173 | G    |
| 36  | 1     | 187 | A    |
| 36  | 1     | 190 | U    |
| 36  | 1     | 191 | U    |
| 36  | 1     | 192 | C    |
| 36  | 1     | 210 | U    |
| 36  | 1     | 211 | A    |
| 36  | 1     | 218 | G    |
| 36  | 1     | 219 | A    |
| 36  | 1     | 224 | C    |
| 36  | 1     | 234 | G    |
| 36  | 1     | 238 | A    |
| 36  | 1     | 240 | U    |
| 36  | 1     | 241 | G    |
| 36  | 1     | 243 | G    |
| 36  | 1     | 245 | U    |
| 36  | 1     | 249 | U    |
| 36  | 1     | 250 | U    |
| 36  | 1     | 251 | G    |
| 36  | 1     | 252 | U    |
| 36  | 1     | 256 | G    |
| 36  | 1     | 269 | G    |
| 36  | 1     | 282 | G    |
| 36  | 1     | 283 | G    |
| 36  | 1     | 286 | U    |
| 36  | 1     | 295 | A    |
| 36  | 1     | 298 | U    |
| 36  | 1     | 305 | U    |
| 36  | 1     | 323 | A    |
| 36  | 1     | 329 | U    |
| 36  | 1     | 344 | A    |
| 36  | 1     | 349 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 1     | 350 | C    |
| 36  | 1     | 352 | A    |
| 36  | 1     | 375 | A    |
| 36  | 1     | 376 | G    |
| 36  | 1     | 395 | A    |
| 36  | 1     | 397 | A    |
| 36  | 1     | 398 | A    |
| 36  | 1     | 401 | U    |
| 36  | 1     | 402 | A    |
| 36  | 1     | 403 | C    |
| 36  | 1     | 417 | A    |
| 36  | 1     | 421 | G    |
| 36  | 1     | 422 | A    |
| 36  | 1     | 438 | A    |
| 36  | 1     | 440 | A    |
| 36  | 1     | 495 | G    |
| 36  | 1     | 520 | U    |
| 36  | 1     | 521 | A    |
| 36  | 1     | 535 | G    |
| 36  | 1     | 544 | C    |
| 36  | 1     | 546 | C    |
| 36  | 1     | 547 | G    |
| 36  | 1     | 548 | G    |
| 36  | 1     | 551 | A    |
| 36  | 1     | 552 | G    |
| 36  | 1     | 555 | U    |
| 36  | 1     | 557 | A    |
| 36  | 1     | 559 | A    |
| 36  | 1     | 578 | A    |
| 36  | 1     | 579 | G    |
| 36  | 1     | 588 | G    |
| 36  | 1     | 589 | A    |
| 36  | 1     | 592 | A    |
| 36  | 1     | 604 | G    |
| 36  | 1     | 609 | G    |
| 36  | 1     | 611 | A    |
| 36  | 1     | 620 | U    |
| 36  | 1     | 621 | A    |
| 36  | 1     | 622 | A    |
| 36  | 1     | 636 | C    |
| 36  | 1     | 637 | C    |
| 36  | 1     | 638 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 1     | 649 | A    |
| 36  | 1     | 654 | C    |
| 36  | 1     | 656 | A    |
| 36  | 1     | 660 | A    |
| 36  | 1     | 677 | A    |
| 36  | 1     | 681 | U    |
| 36  | 1     | 691 | A    |
| 36  | 1     | 705 | A    |
| 36  | 1     | 708 | G    |
| 36  | 1     | 712 | G    |
| 36  | 1     | 715 | A    |
| 36  | 1     | 716 | A    |
| 36  | 1     | 719 | U    |
| 36  | 1     | 720 | A    |
| 36  | 1     | 763 | G    |
| 36  | 1     | 764 | U    |
| 36  | 1     | 765 | C    |
| 36  | 1     | 766 | U    |
| 36  | 1     | 767 | U    |
| 36  | 1     | 776 | U    |
| 36  | 1     | 777 | U    |
| 36  | 1     | 781 | G    |
| 36  | 1     | 785 | G    |
| 36  | 1     | 806 | A    |
| 36  | 1     | 816 | A    |
| 36  | 1     | 817 | A    |
| 36  | 1     | 830 | A    |
| 36  | 1     | 849 | C    |
| 36  | 1     | 861 | C    |
| 36  | 1     | 870 | G    |
| 36  | 1     | 874 | U    |
| 36  | 1     | 879 | U    |
| 36  | 1     | 883 | A    |
| 36  | 1     | 889 | U    |
| 36  | 1     | 890 | C    |
| 36  | 1     | 896 | A    |
| 36  | 1     | 897 | U    |
| 36  | 1     | 907 | G    |
| 36  | 1     | 908 | G    |
| 36  | 1     | 914 | A    |
| 36  | 1     | 916 | G    |
| 36  | 1     | 917 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 921  | A    |
| 36  | 1     | 924  | G    |
| 36  | 1     | 937  | G    |
| 36  | 1     | 943  | U    |
| 36  | 1     | 944  | C    |
| 36  | 1     | 959  | C    |
| 36  | 1     | 960  | U    |
| 36  | 1     | 961  | C    |
| 36  | 1     | 962  | A    |
| 36  | 1     | 966  | U    |
| 36  | 1     | 974  | G    |
| 36  | 1     | 979  | U    |
| 36  | 1     | 980  | A    |
| 36  | 1     | 981  | U    |
| 36  | 1     | 982  | C    |
| 36  | 1     | 993  | G    |
| 36  | 1     | 994  | G    |
| 36  | 1     | 1001 | G    |
| 36  | 1     | 1002 | A    |
| 36  | 1     | 1006 | A    |
| 36  | 1     | 1010 | G    |
| 36  | 1     | 1013 | G    |
| 36  | 1     | 1017 | C    |
| 36  | 1     | 1018 | G    |
| 36  | 1     | 1020 | G    |
| 36  | 1     | 1024 | G    |
| 36  | 1     | 1025 | A    |
| 36  | 1     | 1029 | G    |
| 36  | 1     | 1036 | A    |
| 36  | 1     | 1047 | A    |
| 36  | 1     | 1049 | C    |
| 36  | 1     | 1052 | U    |
| 36  | 1     | 1064 | A    |
| 36  | 1     | 1065 | A    |
| 36  | 1     | 1071 | U    |
| 36  | 1     | 1072 | G    |
| 36  | 1     | 1079 | A    |
| 36  | 1     | 1081 | U    |
| 36  | 1     | 1082 | U    |
| 36  | 1     | 1083 | G    |
| 36  | 1     | 1093 | A    |
| 36  | 1     | 1094 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 1095 | U    |
| 36  | 1     | 1097 | G    |
| 36  | 1     | 1098 | A    |
| 36  | 1     | 1103 | A    |
| 36  | 1     | 1104 | G    |
| 36  | 1     | 1117 | G    |
| 36  | 1     | 1121 | U    |
| 36  | 1     | 1131 | G    |
| 36  | 1     | 1153 | A    |
| 36  | 1     | 1159 | A    |
| 36  | 1     | 1180 | A    |
| 36  | 1     | 1181 | U    |
| 36  | 1     | 1182 | A    |
| 36  | 1     | 1191 | U    |
| 36  | 1     | 1192 | C    |
| 36  | 1     | 1196 | C    |
| 36  | 1     | 1197 | A    |
| 36  | 1     | 1201 | C    |
| 36  | 1     | 1202 | A    |
| 36  | 1     | 1209 | G    |
| 36  | 1     | 1217 | A    |
| 36  | 1     | 1218 | U    |
| 36  | 1     | 1222 | G    |
| 36  | 1     | 1225 | A    |
| 36  | 1     | 1226 | G    |
| 36  | 1     | 1227 | C    |
| 36  | 1     | 1232 | C    |
| 36  | 1     | 1233 | G    |
| 36  | 1     | 1235 | U    |
| 36  | 1     | 1236 | G    |
| 36  | 1     | 1237 | G    |
| 36  | 1     | 1239 | C    |
| 36  | 1     | 1241 | U    |
| 36  | 1     | 1243 | G    |
| 36  | 1     | 1245 | A    |
| 36  | 1     | 1246 | G    |
| 36  | 1     | 1248 | C    |
| 36  | 1     | 1249 | G    |
| 36  | 1     | 1258 | U    |
| 36  | 1     | 1262 | G    |
| 36  | 1     | 1263 | A    |
| 36  | 1     | 1264 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 1265 | U    |
| 36  | 1     | 1266 | G    |
| 36  | 1     | 1269 | U    |
| 36  | 1     | 1270 | A    |
| 36  | 1     | 1271 | A    |
| 36  | 1     | 1274 | A    |
| 36  | 1     | 1278 | A    |
| 36  | 1     | 1279 | C    |
| 36  | 1     | 1280 | C    |
| 36  | 1     | 1285 | G    |
| 36  | 1     | 1287 | A    |
| 36  | 1     | 1292 | C    |
| 36  | 1     | 1307 | G    |
| 36  | 1     | 1308 | A    |
| 36  | 1     | 1309 | U    |
| 36  | 1     | 1313 | G    |
| 36  | 1     | 1317 | A    |
| 36  | 1     | 1318 | A    |
| 36  | 1     | 1329 | U    |
| 36  | 1     | 1330 | A    |
| 36  | 1     | 1348 | U    |
| 36  | 1     | 1349 | G    |
| 36  | 1     | 1350 | A    |
| 36  | 1     | 1351 | U    |
| 36  | 1     | 1352 | A    |
| 36  | 1     | 1353 | U    |
| 36  | 1     | 1355 | A    |
| 36  | 1     | 1356 | U    |
| 36  | 1     | 1357 | G    |
| 36  | 1     | 1380 | G    |
| 36  | 1     | 1386 | A    |
| 36  | 1     | 1399 | A    |
| 36  | 1     | 1400 | G    |
| 36  | 1     | 1419 | A    |
| 36  | 1     | 1422 | G    |
| 36  | 1     | 1434 | G    |
| 36  | 1     | 1437 | C    |
| 36  | 1     | 1445 | U    |
| 36  | 1     | 1446 | A    |
| 36  | 1     | 1449 | A    |
| 36  | 1     | 1450 | G    |
| 36  | 1     | 1481 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 1482 | A    |
| 36  | 1     | 1484 | U    |
| 36  | 1     | 1485 | G    |
| 36  | 1     | 1489 | A    |
| 36  | 1     | 1496 | C    |
| 36  | 1     | 1503 | A    |
| 36  | 1     | 1507 | G    |
| 36  | 1     | 1508 | C    |
| 36  | 1     | 1526 | U    |
| 36  | 1     | 1527 | C    |
| 36  | 1     | 1555 | U    |
| 36  | 1     | 1556 | C    |
| 36  | 1     | 1557 | A    |
| 36  | 1     | 1560 | G    |
| 36  | 1     | 1562 | C    |
| 36  | 1     | 1563 | C    |
| 36  | 1     | 1564 | U    |
| 36  | 1     | 1566 | A    |
| 36  | 1     | 1567 | U    |
| 36  | 1     | 1568 | U    |
| 36  | 1     | 1569 | U    |
| 36  | 1     | 1570 | U    |
| 36  | 1     | 1576 | G    |
| 36  | 1     | 1578 | C    |
| 36  | 1     | 1579 | C    |
| 36  | 1     | 1580 | A    |
| 36  | 1     | 1582 | C    |
| 36  | 1     | 1583 | A    |
| 36  | 1     | 1587 | A    |
| 36  | 1     | 1589 | A    |
| 36  | 1     | 1593 | A    |
| 36  | 1     | 1605 | A    |
| 36  | 1     | 1607 | U    |
| 36  | 1     | 1608 | C    |
| 36  | 1     | 1612 | A    |
| 36  | 1     | 1620 | U    |
| 36  | 1     | 1629 | U    |
| 36  | 1     | 1633 | C    |
| 36  | 1     | 1643 | A    |
| 36  | 1     | 1657 | C    |
| 36  | 1     | 1658 | G    |
| 36  | 1     | 1683 | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 1716 | U    |
| 36  | 1     | 1717 | U    |
| 36  | 1     | 1724 | U    |
| 36  | 1     | 1725 | C    |
| 36  | 1     | 1741 | A    |
| 36  | 1     | 1742 | U    |
| 36  | 1     | 1750 | A    |
| 36  | 1     | 1751 | G    |
| 36  | 1     | 1760 | A    |
| 36  | 1     | 1761 | C    |
| 36  | 1     | 1762 | C    |
| 36  | 1     | 1764 | U    |
| 36  | 1     | 1765 | U    |
| 36  | 1     | 1767 | C    |
| 36  | 1     | 1768 | U    |
| 36  | 1     | 1770 | G    |
| 36  | 1     | 1780 | G    |
| 36  | 1     | 1781 | C    |
| 36  | 1     | 1797 | A    |
| 36  | 1     | 1809 | A    |
| 36  | 1     | 1810 | A    |
| 36  | 1     | 1812 | G    |
| 36  | 1     | 1814 | A    |
| 36  | 1     | 1816 | A    |
| 36  | 1     | 1817 | G    |
| 36  | 1     | 1819 | U    |
| 36  | 1     | 1820 | U    |
| 36  | 1     | 1821 | U    |
| 36  | 1     | 1835 | A    |
| 36  | 1     | 1839 | A    |
| 36  | 1     | 1841 | A    |
| 36  | 1     | 1842 | A    |
| 36  | 1     | 1846 | C    |
| 36  | 1     | 1849 | C    |
| 36  | 1     | 1855 | U    |
| 36  | 1     | 1879 | A    |
| 36  | 1     | 1880 | U    |
| 36  | 1     | 1901 | A    |
| 36  | 1     | 1906 | G    |
| 36  | 1     | 1951 | C    |
| 36  | 1     | 1952 | G    |
| 36  | 1     | 1954 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 2094 | C    |
| 36  | 1     | 2101 | C    |
| 36  | 1     | 2102 | U    |
| 36  | 1     | 2106 | A    |
| 36  | 1     | 2107 | A    |
| 36  | 1     | 2111 | G    |
| 36  | 1     | 2112 | U    |
| 36  | 1     | 2113 | A    |
| 36  | 1     | 2121 | G    |
| 36  | 1     | 2122 | G    |
| 36  | 1     | 2125 | A    |
| 36  | 1     | 2130 | G    |
| 36  | 1     | 2131 | A    |
| 36  | 1     | 2140 | U    |
| 36  | 1     | 2158 | A    |
| 36  | 1     | 2169 | G    |
| 36  | 1     | 2201 | G    |
| 36  | 1     | 2205 | U    |
| 36  | 1     | 2208 | A    |
| 36  | 1     | 2210 | G    |
| 36  | 1     | 2223 | A    |
| 36  | 1     | 2228 | A    |
| 36  | 1     | 2244 | A    |
| 36  | 1     | 2249 | G    |
| 36  | 1     | 2250 | G    |
| 36  | 1     | 2255 | A    |
| 36  | 1     | 2256 | A    |
| 36  | 1     | 2272 | G    |
| 36  | 1     | 2273 | G    |
| 36  | 1     | 2279 | A    |
| 36  | 1     | 2281 | A    |
| 36  | 1     | 2282 | U    |
| 36  | 1     | 2284 | C    |
| 36  | 1     | 2288 | G    |
| 36  | 1     | 2298 | U    |
| 36  | 1     | 2299 | A    |
| 36  | 1     | 2307 | G    |
| 36  | 1     | 2308 | C    |
| 36  | 1     | 2310 | U    |
| 36  | 1     | 2313 | A    |
| 36  | 1     | 2314 | U    |
| 36  | 1     | 2315 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 2319 | U    |
| 36  | 1     | 2334 | U    |
| 36  | 1     | 2336 | U    |
| 36  | 1     | 2366 | C    |
| 36  | 1     | 2372 | A    |
| 36  | 1     | 2373 | A    |
| 36  | 1     | 2374 | C    |
| 36  | 1     | 2375 | G    |
| 36  | 1     | 2385 | G    |
| 36  | 1     | 2388 | U    |
| 36  | 1     | 2393 | G    |
| 36  | 1     | 2397 | A    |
| 36  | 1     | 2401 | A    |
| 36  | 1     | 2402 | A    |
| 36  | 1     | 2403 | G    |
| 36  | 1     | 2404 | A    |
| 36  | 1     | 2405 | C    |
| 36  | 1     | 2411 | U    |
| 36  | 1     | 2412 | G    |
| 36  | 1     | 2418 | G    |
| 36  | 1     | 2419 | A    |
| 36  | 1     | 2435 | G    |
| 36  | 1     | 2437 | G    |
| 36  | 1     | 2444 | C    |
| 36  | 1     | 2445 | A    |
| 36  | 1     | 2502 | A    |
| 36  | 1     | 2503 | G    |
| 36  | 1     | 2513 | U    |
| 36  | 1     | 2514 | U    |
| 36  | 1     | 2515 | A    |
| 36  | 1     | 2519 | A    |
| 36  | 1     | 2522 | G    |
| 36  | 1     | 2523 | A    |
| 36  | 1     | 2529 | A    |
| 36  | 1     | 2532 | U    |
| 36  | 1     | 2537 | U    |
| 36  | 1     | 2538 | U    |
| 36  | 1     | 2539 | C    |
| 36  | 1     | 2540 | A    |
| 36  | 1     | 2541 | U    |
| 36  | 1     | 2542 | U    |
| 36  | 1     | 2543 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 2544 | U    |
| 36  | 1     | 2547 | A    |
| 36  | 1     | 2548 | C    |
| 36  | 1     | 2549 | G    |
| 36  | 1     | 2552 | C    |
| 36  | 1     | 2554 | A    |
| 36  | 1     | 2555 | G    |
| 36  | 1     | 2561 | A    |
| 36  | 1     | 2568 | C    |
| 36  | 1     | 2569 | A    |
| 36  | 1     | 2570 | U    |
| 36  | 1     | 2571 | U    |
| 36  | 1     | 2572 | C    |
| 36  | 1     | 2573 | G    |
| 36  | 1     | 2585 | G    |
| 36  | 1     | 2586 | G    |
| 36  | 1     | 2591 | A    |
| 36  | 1     | 2593 | A    |
| 36  | 1     | 2594 | C    |
| 36  | 1     | 2600 | C    |
| 36  | 1     | 2606 | G    |
| 36  | 1     | 2607 | G    |
| 36  | 1     | 2614 | G    |
| 36  | 1     | 2617 | U    |
| 36  | 1     | 2637 | A    |
| 36  | 1     | 2652 | U    |
| 36  | 1     | 2656 | A    |
| 36  | 1     | 2672 | G    |
| 36  | 1     | 2674 | A    |
| 36  | 1     | 2677 | G    |
| 36  | 1     | 2681 | U    |
| 36  | 1     | 2689 | A    |
| 36  | 1     | 2690 | G    |
| 36  | 1     | 2691 | A    |
| 36  | 1     | 2694 | A    |
| 36  | 1     | 2709 | C    |
| 36  | 1     | 2712 | U    |
| 36  | 1     | 2714 | G    |
| 36  | 1     | 2728 | G    |
| 36  | 1     | 2729 | U    |
| 36  | 1     | 2752 | U    |
| 36  | 1     | 2753 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 2762 | A    |
| 36  | 1     | 2771 | U    |
| 36  | 1     | 2772 | C    |
| 36  | 1     | 2777 | G    |
| 36  | 1     | 2778 | G    |
| 36  | 1     | 2796 | G    |
| 36  | 1     | 2799 | A    |
| 36  | 1     | 2800 | G    |
| 36  | 1     | 2801 | A    |
| 36  | 1     | 2802 | A    |
| 36  | 1     | 2803 | A    |
| 36  | 1     | 2810 | C    |
| 36  | 1     | 2817 | A    |
| 36  | 1     | 2818 | U    |
| 36  | 1     | 2819 | A    |
| 36  | 1     | 2830 | G    |
| 36  | 1     | 2838 | A    |
| 36  | 1     | 2842 | U    |
| 36  | 1     | 2843 | U    |
| 36  | 1     | 2845 | A    |
| 36  | 1     | 2849 | C    |
| 36  | 1     | 2860 | U    |
| 36  | 1     | 2867 | C    |
| 36  | 1     | 2871 | G    |
| 36  | 1     | 2872 | A    |
| 36  | 1     | 2873 | U    |
| 36  | 1     | 2874 | G    |
| 36  | 1     | 2875 | U    |
| 36  | 1     | 2887 | A    |
| 36  | 1     | 2896 | A    |
| 36  | 1     | 2897 | A    |
| 36  | 1     | 2898 | G    |
| 36  | 1     | 2899 | C    |
| 36  | 1     | 2900 | A    |
| 36  | 1     | 2902 | A    |
| 36  | 1     | 2914 | G    |
| 36  | 1     | 2923 | U    |
| 36  | 1     | 2935 | U    |
| 36  | 1     | 2936 | A    |
| 36  | 1     | 2942 | C    |
| 36  | 1     | 2945 | G    |
| 36  | 1     | 2947 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 2957 | G    |
| 36  | 1     | 2971 | A    |
| 36  | 1     | 2974 | U    |
| 36  | 1     | 2980 | U    |
| 36  | 1     | 2983 | C    |
| 36  | 1     | 2990 | G    |
| 36  | 1     | 2996 | U    |
| 36  | 1     | 2997 | G    |
| 36  | 1     | 3012 | A    |
| 36  | 1     | 3049 | A    |
| 36  | 1     | 3056 | U    |
| 36  | 1     | 3057 | U    |
| 36  | 1     | 3058 | U    |
| 36  | 1     | 3059 | G    |
| 36  | 1     | 3078 | U    |
| 36  | 1     | 3079 | U    |
| 36  | 1     | 3086 | A    |
| 36  | 1     | 3092 | C    |
| 36  | 1     | 3113 | A    |
| 36  | 1     | 3122 | A    |
| 36  | 1     | 3128 | G    |
| 36  | 1     | 3130 | A    |
| 36  | 1     | 3131 | U    |
| 36  | 1     | 3134 | A    |
| 36  | 1     | 3142 | A    |
| 36  | 1     | 3143 | C    |
| 36  | 1     | 3151 | U    |
| 36  | 1     | 3153 | U    |
| 36  | 1     | 3154 | C    |
| 36  | 1     | 3155 | U    |
| 36  | 1     | 3156 | U    |
| 36  | 1     | 3157 | U    |
| 36  | 1     | 3158 | G    |
| 36  | 1     | 3164 | C    |
| 36  | 1     | 3165 | A    |
| 36  | 1     | 3170 | A    |
| 36  | 1     | 3171 | U    |
| 36  | 1     | 3173 | G    |
| 36  | 1     | 3174 | A    |
| 36  | 1     | 3176 | G    |
| 36  | 1     | 3179 | U    |
| 36  | 1     | 3180 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 3181 | C    |
| 36  | 1     | 3187 | A    |
| 36  | 1     | 3196 | U    |
| 36  | 1     | 3198 | U    |
| 36  | 1     | 3207 | U    |
| 36  | 1     | 3217 | C    |
| 36  | 1     | 3218 | A    |
| 36  | 1     | 3219 | G    |
| 36  | 1     | 3229 | G    |
| 36  | 1     | 3235 | C    |
| 36  | 1     | 3243 | A    |
| 36  | 1     | 3245 | A    |
| 36  | 1     | 3246 | G    |
| 36  | 1     | 3247 | G    |
| 36  | 1     | 3253 | G    |
| 36  | 1     | 3259 | U    |
| 36  | 1     | 3270 | U    |
| 36  | 1     | 3272 | C    |
| 36  | 1     | 3273 | A    |
| 36  | 1     | 3276 | G    |
| 36  | 1     | 3281 | U    |
| 36  | 1     | 3286 | G    |
| 36  | 1     | 3287 | U    |
| 36  | 1     | 3288 | G    |
| 36  | 1     | 3289 | G    |
| 36  | 1     | 3292 | A    |
| 36  | 1     | 3294 | A    |
| 36  | 1     | 3295 | A    |
| 36  | 1     | 3304 | U    |
| 36  | 1     | 3313 | U    |
| 36  | 1     | 3316 | A    |
| 36  | 1     | 3317 | U    |
| 36  | 1     | 3318 | G    |
| 36  | 1     | 3319 | U    |
| 36  | 1     | 3320 | A    |
| 36  | 1     | 3330 | A    |
| 36  | 1     | 3335 | A    |
| 36  | 1     | 3341 | U    |
| 36  | 1     | 3342 | A    |
| 36  | 1     | 3345 | G    |
| 36  | 1     | 3347 | A    |
| 36  | 1     | 3350 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 3351 | U    |
| 36  | 1     | 3352 | U    |
| 36  | 1     | 3353 | G    |
| 36  | 1     | 3354 | U    |
| 36  | 1     | 3355 | U    |
| 36  | 1     | 3356 | G    |
| 36  | 1     | 3369 | G    |
| 36  | 1     | 3375 | A    |
| 36  | 1     | 3376 | A    |
| 36  | 1     | 3377 | G    |
| 36  | 1     | 3378 | C    |
| 36  | 1     | 3382 | U    |
| 36  | 1     | 3383 | G    |
| 36  | 1     | 3389 | U    |
| 37  | 3     | 7    | G    |
| 37  | 3     | 13   | A    |
| 37  | 3     | 14   | U    |
| 37  | 3     | 22   | A    |
| 37  | 3     | 42   | A    |
| 37  | 3     | 50   | U    |
| 37  | 3     | 51   | A    |
| 37  | 3     | 54   | U    |
| 37  | 3     | 59   | U    |
| 37  | 3     | 65   | G    |
| 37  | 3     | 74   | C    |
| 37  | 3     | 76   | A    |
| 37  | 3     | 95   | A    |
| 37  | 3     | 102  | A    |
| 37  | 3     | 110  | G    |
| 37  | 3     | 112  | G    |
| 37  | 3     | 121  | U    |
| 38  | 4     | 2    | A    |
| 38  | 4     | 11   | C    |
| 38  | 4     | 22   | U    |
| 38  | 4     | 34   | U    |
| 38  | 4     | 35   | C    |
| 38  | 4     | 52   | A    |
| 38  | 4     | 53   | A    |
| 38  | 4     | 59   | A    |
| 38  | 4     | 62   | C    |
| 38  | 4     | 63   | G    |
| 38  | 4     | 79   | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | 4     | 80  | A    |
| 38  | 4     | 81  | U    |
| 38  | 4     | 82  | U    |
| 38  | 4     | 83  | C    |
| 38  | 4     | 84  | C    |
| 38  | 4     | 85  | G    |
| 38  | 4     | 86  | U    |
| 38  | 4     | 87  | G    |
| 38  | 4     | 90  | U    |
| 38  | 4     | 95  | G    |
| 38  | 4     | 96  | A    |
| 38  | 4     | 104 | A    |
| 38  | 4     | 105 | A    |
| 38  | 4     | 106 | C    |
| 38  | 4     | 111 | A    |
| 38  | 4     | 112 | U    |
| 38  | 4     | 113 | U    |
| 38  | 4     | 125 | U    |
| 38  | 4     | 126 | A    |
| 38  | 4     | 128 | U    |
| 38  | 4     | 138 | A    |
| 38  | 4     | 142 | C    |
| 38  | 4     | 152 | G    |
| 38  | 4     | 157 | U    |
| 38  | 4     | 158 | U    |
| 1   | 6     | 2   | A    |
| 1   | 6     | 4   | C    |
| 1   | 6     | 13  | C    |
| 1   | 6     | 25  | C    |
| 1   | 6     | 26  | A    |
| 1   | 6     | 27  | U    |
| 1   | 6     | 34  | G    |
| 1   | 6     | 42  | G    |
| 1   | 6     | 44  | U    |
| 1   | 6     | 46  | A    |
| 1   | 6     | 47  | A    |
| 1   | 6     | 49  | C    |
| 1   | 6     | 50  | C    |
| 1   | 6     | 57  | G    |
| 1   | 6     | 60  | U    |
| 1   | 6     | 67  | A    |
| 1   | 6     | 68  | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 69  | G    |
| 1   | 6     | 72  | A    |
| 1   | 6     | 73  | U    |
| 1   | 6     | 75  | U    |
| 1   | 6     | 76  | A    |
| 1   | 6     | 77  | U    |
| 1   | 6     | 78  | A    |
| 1   | 6     | 100 | A    |
| 1   | 6     | 103 | A    |
| 1   | 6     | 104 | A    |
| 1   | 6     | 114 | C    |
| 1   | 6     | 115 | G    |
| 1   | 6     | 137 | U    |
| 1   | 6     | 138 | A    |
| 1   | 6     | 140 | A    |
| 1   | 6     | 141 | U    |
| 1   | 6     | 144 | U    |
| 1   | 6     | 145 | A    |
| 1   | 6     | 146 | U    |
| 1   | 6     | 153 | G    |
| 1   | 6     | 158 | U    |
| 1   | 6     | 159 | U    |
| 1   | 6     | 166 | C    |
| 1   | 6     | 178 | U    |
| 1   | 6     | 179 | A    |
| 1   | 6     | 185 | U    |
| 1   | 6     | 188 | A    |
| 1   | 6     | 190 | C    |
| 1   | 6     | 191 | C    |
| 1   | 6     | 192 | U    |
| 1   | 6     | 193 | U    |
| 1   | 6     | 195 | G    |
| 1   | 6     | 197 | A    |
| 1   | 6     | 199 | G    |
| 1   | 6     | 200 | A    |
| 1   | 6     | 215 | A    |
| 1   | 6     | 216 | U    |
| 1   | 6     | 217 | A    |
| 1   | 6     | 218 | A    |
| 1   | 6     | 219 | A    |
| 1   | 6     | 220 | A    |
| 1   | 6     | 226 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 227 | U    |
| 1   | 6     | 228 | G    |
| 1   | 6     | 230 | C    |
| 1   | 6     | 232 | U    |
| 1   | 6     | 233 | C    |
| 1   | 6     | 240 | U    |
| 1   | 6     | 241 | U    |
| 1   | 6     | 249 | U    |
| 1   | 6     | 250 | C    |
| 1   | 6     | 261 | U    |
| 1   | 6     | 262 | U    |
| 1   | 6     | 265 | A    |
| 1   | 6     | 271 | A    |
| 1   | 6     | 272 | U    |
| 1   | 6     | 273 | G    |
| 1   | 6     | 275 | C    |
| 1   | 6     | 277 | U    |
| 1   | 6     | 278 | U    |
| 1   | 6     | 280 | U    |
| 1   | 6     | 299 | A    |
| 1   | 6     | 308 | C    |
| 1   | 6     | 314 | C    |
| 1   | 6     | 316 | A    |
| 1   | 6     | 319 | U    |
| 1   | 6     | 321 | C    |
| 1   | 6     | 322 | G    |
| 1   | 6     | 337 | G    |
| 1   | 6     | 338 | C    |
| 1   | 6     | 352 | A    |
| 1   | 6     | 353 | A    |
| 1   | 6     | 359 | A    |
| 1   | 6     | 360 | A    |
| 1   | 6     | 361 | C    |
| 1   | 6     | 370 | A    |
| 1   | 6     | 393 | C    |
| 1   | 6     | 400 | A    |
| 1   | 6     | 401 | A    |
| 1   | 6     | 402 | C    |
| 1   | 6     | 404 | G    |
| 1   | 6     | 416 | A    |
| 1   | 6     | 417 | A    |
| 1   | 6     | 418 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 424 | C    |
| 1   | 6     | 425 | A    |
| 1   | 6     | 426 | G    |
| 1   | 6     | 434 | G    |
| 1   | 6     | 439 | U    |
| 1   | 6     | 444 | C    |
| 1   | 6     | 445 | A    |
| 1   | 6     | 448 | C    |
| 1   | 6     | 454 | U    |
| 1   | 6     | 468 | A    |
| 1   | 6     | 469 | C    |
| 1   | 6     | 470 | A    |
| 1   | 6     | 475 | A    |
| 1   | 6     | 477 | A    |
| 1   | 6     | 484 | C    |
| 1   | 6     | 486 | G    |
| 1   | 6     | 487 | G    |
| 1   | 6     | 488 | G    |
| 1   | 6     | 489 | C    |
| 1   | 6     | 490 | C    |
| 1   | 6     | 492 | A    |
| 1   | 6     | 493 | U    |
| 1   | 6     | 494 | U    |
| 1   | 6     | 495 | C    |
| 1   | 6     | 496 | G    |
| 1   | 6     | 497 | G    |
| 1   | 6     | 500 | C    |
| 1   | 6     | 501 | U    |
| 1   | 6     | 504 | U    |
| 1   | 6     | 505 | A    |
| 1   | 6     | 506 | A    |
| 1   | 6     | 507 | U    |
| 1   | 6     | 508 | U    |
| 1   | 6     | 510 | G    |
| 1   | 6     | 511 | A    |
| 1   | 6     | 512 | A    |
| 1   | 6     | 513 | U    |
| 1   | 6     | 514 | G    |
| 1   | 6     | 519 | C    |
| 1   | 6     | 527 | A    |
| 1   | 6     | 534 | A    |
| 1   | 6     | 538 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 539 | G    |
| 1   | 6     | 540 | G    |
| 1   | 6     | 541 | A    |
| 1   | 6     | 542 | A    |
| 1   | 6     | 543 | C    |
| 1   | 6     | 544 | A    |
| 1   | 6     | 548 | G    |
| 1   | 6     | 555 | A    |
| 1   | 6     | 557 | G    |
| 1   | 6     | 558 | U    |
| 1   | 6     | 559 | C    |
| 1   | 6     | 565 | C    |
| 1   | 6     | 570 | A    |
| 1   | 6     | 574 | G    |
| 1   | 6     | 579 | A    |
| 1   | 6     | 580 | A    |
| 1   | 6     | 582 | U    |
| 1   | 6     | 594 | A    |
| 1   | 6     | 595 | G    |
| 1   | 6     | 606 | A    |
| 1   | 6     | 609 | U    |
| 1   | 6     | 610 | G    |
| 1   | 6     | 617 | U    |
| 1   | 6     | 619 | A    |
| 1   | 6     | 620 | A    |
| 1   | 6     | 622 | A    |
| 1   | 6     | 623 | A    |
| 1   | 6     | 624 | G    |
| 1   | 6     | 630 | A    |
| 1   | 6     | 637 | C    |
| 1   | 6     | 639 | U    |
| 1   | 6     | 640 | U    |
| 1   | 6     | 652 | G    |
| 1   | 6     | 653 | C    |
| 1   | 6     | 658 | C    |
| 1   | 6     | 661 | A    |
| 1   | 6     | 662 | U    |
| 1   | 6     | 665 | U    |
| 1   | 6     | 667 | U    |
| 1   | 6     | 668 | C    |
| 1   | 6     | 670 | U    |
| 1   | 6     | 676 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 679 | U    |
| 1   | 6     | 681 | U    |
| 1   | 6     | 682 | C    |
| 1   | 6     | 683 | C    |
| 1   | 6     | 684 | A    |
| 1   | 6     | 685 | A    |
| 1   | 6     | 687 | G    |
| 1   | 6     | 689 | G    |
| 1   | 6     | 691 | C    |
| 1   | 6     | 696 | C    |
| 1   | 6     | 710 | U    |
| 1   | 6     | 711 | U    |
| 1   | 6     | 714 | G    |
| 1   | 6     | 718 | U    |
| 1   | 6     | 719 | U    |
| 1   | 6     | 720 | G    |
| 1   | 6     | 721 | U    |
| 1   | 6     | 722 | G    |
| 1   | 6     | 723 | G    |
| 1   | 6     | 730 | G    |
| 1   | 6     | 733 | A    |
| 1   | 6     | 742 | U    |
| 1   | 6     | 753 | A    |
| 1   | 6     | 754 | A    |
| 1   | 6     | 755 | A    |
| 1   | 6     | 756 | A    |
| 1   | 6     | 765 | G    |
| 1   | 6     | 774 | A    |
| 1   | 6     | 775 | G    |
| 1   | 6     | 780 | A    |
| 1   | 6     | 781 | U    |
| 1   | 6     | 782 | U    |
| 1   | 6     | 783 | G    |
| 1   | 6     | 789 | A    |
| 1   | 6     | 793 | A    |
| 1   | 6     | 794 | U    |
| 1   | 6     | 795 | U    |
| 1   | 6     | 806 | A    |
| 1   | 6     | 807 | A    |
| 1   | 6     | 811 | A    |
| 1   | 6     | 812 | A    |
| 1   | 6     | 815 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 821  | U    |
| 1   | 6     | 823  | G    |
| 1   | 6     | 825  | U    |
| 1   | 6     | 826  | U    |
| 1   | 6     | 829  | A    |
| 1   | 6     | 830  | U    |
| 1   | 6     | 831  | U    |
| 1   | 6     | 832  | U    |
| 1   | 6     | 834  | G    |
| 1   | 6     | 835  | U    |
| 1   | 6     | 856  | A    |
| 1   | 6     | 863  | A    |
| 1   | 6     | 864  | U    |
| 1   | 6     | 873  | U    |
| 1   | 6     | 898  | A    |
| 1   | 6     | 906  | A    |
| 1   | 6     | 910  | C    |
| 1   | 6     | 912  | U    |
| 1   | 6     | 913  | G    |
| 1   | 6     | 914  | G    |
| 1   | 6     | 916  | U    |
| 1   | 6     | 933  | A    |
| 1   | 6     | 935  | U    |
| 1   | 6     | 942  | G    |
| 1   | 6     | 959  | U    |
| 1   | 6     | 960  | U    |
| 1   | 6     | 966  | A    |
| 1   | 6     | 969  | C    |
| 1   | 6     | 970  | A    |
| 1   | 6     | 971  | A    |
| 1   | 6     | 991  | G    |
| 1   | 6     | 992  | A    |
| 1   | 6     | 993  | A    |
| 1   | 6     | 996  | U    |
| 1   | 6     | 997  | G    |
| 1   | 6     | 1003 | A    |
| 1   | 6     | 1004 | U    |
| 1   | 6     | 1005 | A    |
| 1   | 6     | 1026 | A    |
| 1   | 6     | 1028 | C    |
| 1   | 6     | 1039 | A    |
| 1   | 6     | 1040 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 1046 | G    |
| 1   | 6     | 1052 | U    |
| 1   | 6     | 1053 | G    |
| 1   | 6     | 1057 | U    |
| 1   | 6     | 1058 | U    |
| 1   | 6     | 1059 | U    |
| 1   | 6     | 1060 | U    |
| 1   | 6     | 1075 | C    |
| 1   | 6     | 1082 | C    |
| 1   | 6     | 1091 | A    |
| 1   | 6     | 1092 | A    |
| 1   | 6     | 1096 | C    |
| 1   | 6     | 1097 | U    |
| 1   | 6     | 1098 | U    |
| 1   | 6     | 1099 | U    |
| 1   | 6     | 1100 | G    |
| 1   | 6     | 1101 | G    |
| 1   | 6     | 1109 | G    |
| 1   | 6     | 1138 | A    |
| 1   | 6     | 1146 | G    |
| 1   | 6     | 1150 | G    |
| 1   | 6     | 1151 | A    |
| 1   | 6     | 1155 | G    |
| 1   | 6     | 1158 | C    |
| 1   | 6     | 1159 | C    |
| 1   | 6     | 1160 | A    |
| 1   | 6     | 1162 | C    |
| 1   | 6     | 1167 | G    |
| 1   | 6     | 1185 | U    |
| 1   | 6     | 1194 | A    |
| 1   | 6     | 1196 | A    |
| 1   | 6     | 1197 | C    |
| 1   | 6     | 1199 | G    |
| 1   | 6     | 1200 | G    |
| 1   | 6     | 1202 | A    |
| 1   | 6     | 1203 | A    |
| 1   | 6     | 1208 | A    |
| 1   | 6     | 1212 | G    |
| 1   | 6     | 1217 | A    |
| 1   | 6     | 1218 | G    |
| 1   | 6     | 1219 | A    |
| 1   | 6     | 1220 | C    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 1226 | A    |
| 1   | 6     | 1228 | G    |
| 1   | 6     | 1229 | G    |
| 1   | 6     | 1230 | A    |
| 1   | 6     | 1231 | U    |
| 1   | 6     | 1239 | U    |
| 1   | 6     | 1241 | G    |
| 1   | 6     | 1243 | G    |
| 1   | 6     | 1244 | A    |
| 1   | 6     | 1245 | G    |
| 1   | 6     | 1246 | C    |
| 1   | 6     | 1255 | G    |
| 1   | 6     | 1256 | A    |
| 1   | 6     | 1257 | U    |
| 1   | 6     | 1258 | U    |
| 1   | 6     | 1259 | U    |
| 1   | 6     | 1284 | C    |
| 1   | 6     | 1285 | U    |
| 1   | 6     | 1286 | U    |
| 1   | 6     | 1288 | G    |
| 1   | 6     | 1314 | U    |
| 1   | 6     | 1315 | U    |
| 1   | 6     | 1316 | G    |
| 1   | 6     | 1321 | A    |
| 1   | 6     | 1330 | G    |
| 1   | 6     | 1338 | C    |
| 1   | 6     | 1344 | A    |
| 1   | 6     | 1345 | A    |
| 1   | 6     | 1346 | A    |
| 1   | 6     | 1354 | G    |
| 1   | 6     | 1361 | U    |
| 1   | 6     | 1363 | U    |
| 1   | 6     | 1364 | G    |
| 1   | 6     | 1370 | U    |
| 1   | 6     | 1371 | A    |
| 1   | 6     | 1388 | A    |
| 1   | 6     | 1390 | U    |
| 1   | 6     | 1398 | U    |
| 1   | 6     | 1399 | C    |
| 1   | 6     | 1400 | A    |
| 1   | 6     | 1402 | G    |
| 1   | 6     | 1412 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 1413 | U    |
| 1   | 6     | 1415 | U    |
| 1   | 6     | 1427 | A    |
| 1   | 6     | 1428 | G    |
| 1   | 6     | 1433 | G    |
| 1   | 6     | 1445 | G    |
| 1   | 6     | 1446 | A    |
| 1   | 6     | 1448 | G    |
| 1   | 6     | 1458 | G    |
| 1   | 6     | 1459 | C    |
| 1   | 6     | 1461 | C    |
| 1   | 6     | 1471 | A    |
| 1   | 6     | 1481 | C    |
| 1   | 6     | 1482 | C    |
| 1   | 6     | 1489 | U    |
| 1   | 6     | 1490 | C    |
| 1   | 6     | 1491 | U    |
| 1   | 6     | 1492 | A    |
| 1   | 6     | 1493 | A    |
| 1   | 6     | 1494 | C    |
| 1   | 6     | 1496 | U    |
| 1   | 6     | 1497 | U    |
| 1   | 6     | 1506 | G    |
| 1   | 6     | 1514 | U    |
| 1   | 6     | 1515 | A    |
| 1   | 6     | 1516 | A    |
| 1   | 6     | 1521 | G    |
| 1   | 6     | 1523 | G    |
| 1   | 6     | 1524 | A    |
| 1   | 6     | 1535 | U    |
| 1   | 6     | 1536 | G    |
| 1   | 6     | 1537 | C    |
| 1   | 6     | 1538 | U    |
| 1   | 6     | 1539 | G    |
| 1   | 6     | 1540 | G    |
| 1   | 6     | 1554 | U    |
| 1   | 6     | 1557 | U    |
| 1   | 6     | 1559 | A    |
| 1   | 6     | 1569 | A    |
| 1   | 6     | 1572 | G    |
| 1   | 6     | 1573 | A    |
| 1   | 6     | 1574 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 1575 | G    |
| 1   | 6     | 1577 | A    |
| 1   | 6     | 1584 | G    |
| 1   | 6     | 1601 | G    |
| 1   | 6     | 1616 | G    |
| 1   | 6     | 1621 | U    |
| 1   | 6     | 1634 | C    |
| 1   | 6     | 1639 | C    |
| 1   | 6     | 1657 | U    |
| 1   | 6     | 1658 | G    |
| 1   | 6     | 1683 | C    |
| 1   | 6     | 1697 | G    |
| 1   | 6     | 1698 | G    |
| 1   | 6     | 1699 | G    |
| 1   | 6     | 1700 | C    |
| 1   | 6     | 1701 | A    |
| 1   | 6     | 1702 | A    |
| 1   | 6     | 1703 | C    |
| 1   | 6     | 1710 | U    |
| 1   | 6     | 1712 | A    |
| 1   | 6     | 1716 | C    |
| 1   | 6     | 1717 | G    |
| 1   | 6     | 1731 | A    |
| 1   | 6     | 1742 | U    |
| 1   | 6     | 1755 | A    |
| 1   | 6     | 1760 | G    |
| 1   | 6     | 1762 | A    |
| 1   | 6     | 1766 | A    |
| 1   | 6     | 1767 | G    |
| 1   | 6     | 1769 | U    |
| 1   | 6     | 1770 | U    |
| 1   | 6     | 1780 | G    |
| 1   | 6     | 1782 | A    |
| 1   | 6     | 1783 | C    |
| 1   | 6     | 1792 | G    |
| 1   | 6     | 1793 | G    |
| 1   | 6     | 1794 | A    |
| 1   | 6     | 1795 | U    |
| 1   | 6     | 1796 | C    |
| 1   | 6     | 1799 | U    |
| 1   | 6     | 1800 | A    |
| 36  | 5     | 11   | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 5     | 15  | C    |
| 36  | 5     | 26  | A    |
| 36  | 5     | 38  | U    |
| 36  | 5     | 40  | A    |
| 36  | 5     | 43  | A    |
| 36  | 5     | 44  | U    |
| 36  | 5     | 49  | A    |
| 36  | 5     | 59  | G    |
| 36  | 5     | 60  | A    |
| 36  | 5     | 65  | A    |
| 36  | 5     | 66  | A    |
| 36  | 5     | 76  | G    |
| 36  | 5     | 99  | A    |
| 36  | 5     | 110 | G    |
| 36  | 5     | 113 | C    |
| 36  | 5     | 116 | A    |
| 36  | 5     | 121 | A    |
| 36  | 5     | 122 | A    |
| 36  | 5     | 131 | C    |
| 36  | 5     | 133 | U    |
| 36  | 5     | 134 | U    |
| 36  | 5     | 136 | G    |
| 36  | 5     | 139 | G    |
| 36  | 5     | 150 | A    |
| 36  | 5     | 156 | G    |
| 36  | 5     | 157 | A    |
| 36  | 5     | 165 | A    |
| 36  | 5     | 171 | G    |
| 36  | 5     | 172 | G    |
| 36  | 5     | 173 | G    |
| 36  | 5     | 174 | C    |
| 36  | 5     | 180 | C    |
| 36  | 5     | 182 | U    |
| 36  | 5     | 184 | U    |
| 36  | 5     | 187 | A    |
| 36  | 5     | 190 | U    |
| 36  | 5     | 191 | U    |
| 36  | 5     | 193 | C    |
| 36  | 5     | 204 | A    |
| 36  | 5     | 210 | U    |
| 36  | 5     | 211 | A    |
| 36  | 5     | 218 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 5     | 219 | A    |
| 36  | 5     | 221 | A    |
| 36  | 5     | 222 | A    |
| 36  | 5     | 236 | G    |
| 36  | 5     | 237 | G    |
| 36  | 5     | 238 | A    |
| 36  | 5     | 239 | G    |
| 36  | 5     | 240 | U    |
| 36  | 5     | 244 | G    |
| 36  | 5     | 247 | C    |
| 36  | 5     | 248 | U    |
| 36  | 5     | 249 | U    |
| 36  | 5     | 250 | U    |
| 36  | 5     | 251 | G    |
| 36  | 5     | 252 | U    |
| 36  | 5     | 253 | A    |
| 36  | 5     | 254 | A    |
| 36  | 5     | 259 | C    |
| 36  | 5     | 269 | G    |
| 36  | 5     | 282 | G    |
| 36  | 5     | 283 | G    |
| 36  | 5     | 284 | A    |
| 36  | 5     | 286 | U    |
| 36  | 5     | 295 | A    |
| 36  | 5     | 298 | U    |
| 36  | 5     | 311 | C    |
| 36  | 5     | 322 | U    |
| 36  | 5     | 323 | A    |
| 36  | 5     | 329 | U    |
| 36  | 5     | 349 | A    |
| 36  | 5     | 350 | C    |
| 36  | 5     | 352 | A    |
| 36  | 5     | 376 | G    |
| 36  | 5     | 397 | A    |
| 36  | 5     | 398 | A    |
| 36  | 5     | 399 | A    |
| 36  | 5     | 401 | U    |
| 36  | 5     | 402 | A    |
| 36  | 5     | 403 | C    |
| 36  | 5     | 421 | G    |
| 36  | 5     | 422 | A    |
| 36  | 5     | 436 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 5     | 437 | G    |
| 36  | 5     | 438 | A    |
| 36  | 5     | 439 | C    |
| 36  | 5     | 440 | A    |
| 36  | 5     | 441 | U    |
| 36  | 5     | 442 | G    |
| 36  | 5     | 443 | G    |
| 36  | 5     | 492 | U    |
| 36  | 5     | 495 | G    |
| 36  | 5     | 520 | U    |
| 36  | 5     | 521 | A    |
| 36  | 5     | 535 | G    |
| 36  | 5     | 542 | G    |
| 36  | 5     | 546 | C    |
| 36  | 5     | 547 | G    |
| 36  | 5     | 548 | G    |
| 36  | 5     | 551 | A    |
| 36  | 5     | 555 | U    |
| 36  | 5     | 557 | A    |
| 36  | 5     | 559 | A    |
| 36  | 5     | 560 | G    |
| 36  | 5     | 578 | A    |
| 36  | 5     | 579 | G    |
| 36  | 5     | 592 | A    |
| 36  | 5     | 600 | G    |
| 36  | 5     | 604 | G    |
| 36  | 5     | 609 | G    |
| 36  | 5     | 611 | A    |
| 36  | 5     | 619 | A    |
| 36  | 5     | 620 | U    |
| 36  | 5     | 621 | A    |
| 36  | 5     | 630 | A    |
| 36  | 5     | 636 | C    |
| 36  | 5     | 647 | A    |
| 36  | 5     | 648 | C    |
| 36  | 5     | 649 | A    |
| 36  | 5     | 660 | A    |
| 36  | 5     | 677 | A    |
| 36  | 5     | 681 | U    |
| 36  | 5     | 683 | U    |
| 36  | 5     | 684 | G    |
| 36  | 5     | 705 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 5     | 708 | G    |
| 36  | 5     | 712 | G    |
| 36  | 5     | 715 | A    |
| 36  | 5     | 716 | A    |
| 36  | 5     | 719 | U    |
| 36  | 5     | 720 | A    |
| 36  | 5     | 725 | G    |
| 36  | 5     | 726 | G    |
| 36  | 5     | 727 | G    |
| 36  | 5     | 735 | A    |
| 36  | 5     | 736 | A    |
| 36  | 5     | 758 | C    |
| 36  | 5     | 766 | U    |
| 36  | 5     | 767 | U    |
| 36  | 5     | 768 | C    |
| 36  | 5     | 774 | G    |
| 36  | 5     | 776 | U    |
| 36  | 5     | 777 | U    |
| 36  | 5     | 781 | G    |
| 36  | 5     | 785 | G    |
| 36  | 5     | 786 | A    |
| 36  | 5     | 806 | A    |
| 36  | 5     | 816 | A    |
| 36  | 5     | 817 | A    |
| 36  | 5     | 830 | A    |
| 36  | 5     | 861 | C    |
| 36  | 5     | 874 | U    |
| 36  | 5     | 876 | A    |
| 36  | 5     | 879 | U    |
| 36  | 5     | 891 | G    |
| 36  | 5     | 895 | A    |
| 36  | 5     | 896 | A    |
| 36  | 5     | 897 | U    |
| 36  | 5     | 907 | G    |
| 36  | 5     | 908 | G    |
| 36  | 5     | 914 | A    |
| 36  | 5     | 916 | G    |
| 36  | 5     | 917 | A    |
| 36  | 5     | 921 | A    |
| 36  | 5     | 923 | C    |
| 36  | 5     | 937 | G    |
| 36  | 5     | 944 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 959  | C    |
| 36  | 5     | 960  | U    |
| 36  | 5     | 963  | G    |
| 36  | 5     | 974  | G    |
| 36  | 5     | 979  | U    |
| 36  | 5     | 980  | A    |
| 36  | 5     | 983  | A    |
| 36  | 5     | 993  | G    |
| 36  | 5     | 994  | G    |
| 36  | 5     | 1001 | G    |
| 36  | 5     | 1002 | A    |
| 36  | 5     | 1003 | A    |
| 36  | 5     | 1010 | G    |
| 36  | 5     | 1015 | U    |
| 36  | 5     | 1016 | C    |
| 36  | 5     | 1017 | C    |
| 36  | 5     | 1018 | G    |
| 36  | 5     | 1021 | G    |
| 36  | 5     | 1024 | G    |
| 36  | 5     | 1025 | A    |
| 36  | 5     | 1026 | A    |
| 36  | 5     | 1028 | U    |
| 36  | 5     | 1029 | G    |
| 36  | 5     | 1032 | C    |
| 36  | 5     | 1034 | U    |
| 36  | 5     | 1035 | G    |
| 36  | 5     | 1047 | A    |
| 36  | 5     | 1049 | C    |
| 36  | 5     | 1064 | A    |
| 36  | 5     | 1065 | A    |
| 36  | 5     | 1071 | U    |
| 36  | 5     | 1072 | G    |
| 36  | 5     | 1075 | A    |
| 36  | 5     | 1081 | U    |
| 36  | 5     | 1082 | U    |
| 36  | 5     | 1093 | A    |
| 36  | 5     | 1094 | U    |
| 36  | 5     | 1095 | U    |
| 36  | 5     | 1096 | U    |
| 36  | 5     | 1097 | G    |
| 36  | 5     | 1098 | A    |
| 36  | 5     | 1103 | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1104 | G    |
| 36  | 5     | 1117 | G    |
| 36  | 5     | 1131 | G    |
| 36  | 5     | 1144 | U    |
| 36  | 5     | 1153 | A    |
| 36  | 5     | 1159 | A    |
| 36  | 5     | 1166 | G    |
| 36  | 5     | 1180 | A    |
| 36  | 5     | 1181 | U    |
| 36  | 5     | 1182 | A    |
| 36  | 5     | 1192 | C    |
| 36  | 5     | 1193 | A    |
| 36  | 5     | 1196 | C    |
| 36  | 5     | 1201 | C    |
| 36  | 5     | 1202 | A    |
| 36  | 5     | 1222 | G    |
| 36  | 5     | 1232 | C    |
| 36  | 5     | 1235 | U    |
| 36  | 5     | 1236 | G    |
| 36  | 5     | 1237 | G    |
| 36  | 5     | 1238 | C    |
| 36  | 5     | 1239 | C    |
| 36  | 5     | 1241 | U    |
| 36  | 5     | 1242 | G    |
| 36  | 5     | 1245 | A    |
| 36  | 5     | 1246 | G    |
| 36  | 5     | 1254 | C    |
| 36  | 5     | 1258 | U    |
| 36  | 5     | 1259 | A    |
| 36  | 5     | 1262 | G    |
| 36  | 5     | 1263 | A    |
| 36  | 5     | 1264 | G    |
| 36  | 5     | 1265 | U    |
| 36  | 5     | 1266 | G    |
| 36  | 5     | 1285 | G    |
| 36  | 5     | 1307 | G    |
| 36  | 5     | 1308 | A    |
| 36  | 5     | 1309 | U    |
| 36  | 5     | 1312 | C    |
| 36  | 5     | 1314 | C    |
| 36  | 5     | 1317 | A    |
| 36  | 5     | 1318 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1329 | U    |
| 36  | 5     | 1330 | A    |
| 36  | 5     | 1331 | U    |
| 36  | 5     | 1332 | A    |
| 36  | 5     | 1349 | G    |
| 36  | 5     | 1351 | U    |
| 36  | 5     | 1352 | A    |
| 36  | 5     | 1353 | U    |
| 36  | 5     | 1354 | G    |
| 36  | 5     | 1355 | A    |
| 36  | 5     | 1356 | U    |
| 36  | 5     | 1357 | G    |
| 36  | 5     | 1385 | C    |
| 36  | 5     | 1386 | A    |
| 36  | 5     | 1387 | G    |
| 36  | 5     | 1399 | A    |
| 36  | 5     | 1400 | G    |
| 36  | 5     | 1418 | A    |
| 36  | 5     | 1419 | A    |
| 36  | 5     | 1428 | A    |
| 36  | 5     | 1434 | G    |
| 36  | 5     | 1435 | A    |
| 36  | 5     | 1437 | C    |
| 36  | 5     | 1446 | A    |
| 36  | 5     | 1450 | G    |
| 36  | 5     | 1481 | A    |
| 36  | 5     | 1482 | A    |
| 36  | 5     | 1490 | A    |
| 36  | 5     | 1500 | G    |
| 36  | 5     | 1502 | C    |
| 36  | 5     | 1503 | A    |
| 36  | 5     | 1508 | C    |
| 36  | 5     | 1522 | U    |
| 36  | 5     | 1536 | G    |
| 36  | 5     | 1553 | U    |
| 36  | 5     | 1554 | U    |
| 36  | 5     | 1555 | U    |
| 36  | 5     | 1556 | C    |
| 36  | 5     | 1560 | G    |
| 36  | 5     | 1561 | G    |
| 36  | 5     | 1562 | C    |
| 36  | 5     | 1564 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1565 | G    |
| 36  | 5     | 1566 | A    |
| 36  | 5     | 1567 | U    |
| 36  | 5     | 1569 | U    |
| 36  | 5     | 1570 | U    |
| 36  | 5     | 1571 | A    |
| 36  | 5     | 1572 | U    |
| 36  | 5     | 1574 | C    |
| 36  | 5     | 1575 | A    |
| 36  | 5     | 1576 | G    |
| 36  | 5     | 1577 | G    |
| 36  | 5     | 1578 | C    |
| 36  | 5     | 1579 | C    |
| 36  | 5     | 1581 | C    |
| 36  | 5     | 1582 | C    |
| 36  | 5     | 1583 | A    |
| 36  | 5     | 1587 | A    |
| 36  | 5     | 1589 | A    |
| 36  | 5     | 1593 | A    |
| 36  | 5     | 1605 | A    |
| 36  | 5     | 1620 | U    |
| 36  | 5     | 1629 | U    |
| 36  | 5     | 1638 | A    |
| 36  | 5     | 1639 | C    |
| 36  | 5     | 1643 | A    |
| 36  | 5     | 1644 | C    |
| 36  | 5     | 1645 | U    |
| 36  | 5     | 1655 | G    |
| 36  | 5     | 1657 | C    |
| 36  | 5     | 1658 | G    |
| 36  | 5     | 1683 | A    |
| 36  | 5     | 1685 | C    |
| 36  | 5     | 1686 | U    |
| 36  | 5     | 1687 | U    |
| 36  | 5     | 1716 | U    |
| 36  | 5     | 1717 | U    |
| 36  | 5     | 1724 | U    |
| 36  | 5     | 1725 | C    |
| 36  | 5     | 1741 | A    |
| 36  | 5     | 1750 | A    |
| 36  | 5     | 1751 | G    |
| 36  | 5     | 1762 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1765 | U    |
| 36  | 5     | 1766 | G    |
| 36  | 5     | 1770 | G    |
| 36  | 5     | 1779 | C    |
| 36  | 5     | 1780 | G    |
| 36  | 5     | 1797 | A    |
| 36  | 5     | 1810 | A    |
| 36  | 5     | 1814 | A    |
| 36  | 5     | 1816 | A    |
| 36  | 5     | 1817 | G    |
| 36  | 5     | 1818 | U    |
| 36  | 5     | 1821 | U    |
| 36  | 5     | 1839 | A    |
| 36  | 5     | 1841 | A    |
| 36  | 5     | 1842 | A    |
| 36  | 5     | 1846 | C    |
| 36  | 5     | 1847 | A    |
| 36  | 5     | 1849 | C    |
| 36  | 5     | 1850 | A    |
| 36  | 5     | 1876 | U    |
| 36  | 5     | 1878 | G    |
| 36  | 5     | 1879 | A    |
| 36  | 5     | 1880 | U    |
| 36  | 5     | 1893 | A    |
| 36  | 5     | 1906 | G    |
| 36  | 5     | 1935 | G    |
| 36  | 5     | 1940 | G    |
| 36  | 5     | 1952 | G    |
| 36  | 5     | 1953 | G    |
| 36  | 5     | 2100 | A    |
| 36  | 5     | 2101 | C    |
| 36  | 5     | 2102 | U    |
| 36  | 5     | 2112 | U    |
| 36  | 5     | 2113 | A    |
| 36  | 5     | 2121 | G    |
| 36  | 5     | 2122 | G    |
| 36  | 5     | 2131 | A    |
| 36  | 5     | 2158 | A    |
| 36  | 5     | 2169 | G    |
| 36  | 5     | 2170 | U    |
| 36  | 5     | 2179 | C    |
| 36  | 5     | 2201 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 2205 | U    |
| 36  | 5     | 2206 | G    |
| 36  | 5     | 2210 | G    |
| 36  | 5     | 2223 | A    |
| 36  | 5     | 2228 | A    |
| 36  | 5     | 2244 | A    |
| 36  | 5     | 2250 | G    |
| 36  | 5     | 2251 | G    |
| 36  | 5     | 2253 | G    |
| 36  | 5     | 2255 | A    |
| 36  | 5     | 2256 | A    |
| 36  | 5     | 2257 | C    |
| 36  | 5     | 2258 | U    |
| 36  | 5     | 2269 | U    |
| 36  | 5     | 2273 | G    |
| 36  | 5     | 2279 | A    |
| 36  | 5     | 2281 | A    |
| 36  | 5     | 2288 | G    |
| 36  | 5     | 2306 | C    |
| 36  | 5     | 2307 | G    |
| 36  | 5     | 2310 | U    |
| 36  | 5     | 2313 | A    |
| 36  | 5     | 2315 | G    |
| 36  | 5     | 2334 | U    |
| 36  | 5     | 2335 | G    |
| 36  | 5     | 2336 | U    |
| 36  | 5     | 2360 | C    |
| 36  | 5     | 2372 | A    |
| 36  | 5     | 2373 | A    |
| 36  | 5     | 2374 | C    |
| 36  | 5     | 2375 | G    |
| 36  | 5     | 2385 | G    |
| 36  | 5     | 2393 | G    |
| 36  | 5     | 2394 | G    |
| 36  | 5     | 2396 | G    |
| 36  | 5     | 2397 | A    |
| 36  | 5     | 2398 | A    |
| 36  | 5     | 2399 | A    |
| 36  | 5     | 2401 | A    |
| 36  | 5     | 2402 | A    |
| 36  | 5     | 2403 | G    |
| 36  | 5     | 2404 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 2405 | C    |
| 36  | 5     | 2411 | U    |
| 36  | 5     | 2418 | G    |
| 36  | 5     | 2419 | A    |
| 36  | 5     | 2435 | G    |
| 36  | 5     | 2436 | U    |
| 36  | 5     | 2438 | A    |
| 36  | 5     | 2439 | A    |
| 36  | 5     | 2441 | A    |
| 36  | 5     | 2443 | A    |
| 36  | 5     | 2504 | U    |
| 36  | 5     | 2505 | U    |
| 36  | 5     | 2506 | U    |
| 36  | 5     | 2507 | C    |
| 36  | 5     | 2508 | U    |
| 36  | 5     | 2510 | U    |
| 36  | 5     | 2511 | A    |
| 36  | 5     | 2512 | C    |
| 36  | 5     | 2514 | U    |
| 36  | 5     | 2515 | A    |
| 36  | 5     | 2518 | C    |
| 36  | 5     | 2523 | A    |
| 36  | 5     | 2526 | C    |
| 36  | 5     | 2530 | G    |
| 36  | 5     | 2531 | C    |
| 36  | 5     | 2532 | U    |
| 36  | 5     | 2534 | G    |
| 36  | 5     | 2536 | A    |
| 36  | 5     | 2538 | U    |
| 36  | 5     | 2539 | C    |
| 36  | 5     | 2540 | A    |
| 36  | 5     | 2543 | U    |
| 36  | 5     | 2549 | G    |
| 36  | 5     | 2550 | U    |
| 36  | 5     | 2552 | C    |
| 36  | 5     | 2555 | G    |
| 36  | 5     | 2566 | C    |
| 36  | 5     | 2567 | C    |
| 36  | 5     | 2568 | C    |
| 36  | 5     | 2569 | A    |
| 36  | 5     | 2570 | U    |
| 36  | 5     | 2571 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 2572 | C    |
| 36  | 5     | 2574 | G    |
| 36  | 5     | 2584 | G    |
| 36  | 5     | 2585 | G    |
| 36  | 5     | 2589 | G    |
| 36  | 5     | 2593 | A    |
| 36  | 5     | 2594 | C    |
| 36  | 5     | 2606 | G    |
| 36  | 5     | 2607 | G    |
| 36  | 5     | 2610 | G    |
| 36  | 5     | 2614 | G    |
| 36  | 5     | 2622 | C    |
| 36  | 5     | 2637 | A    |
| 36  | 5     | 2639 | G    |
| 36  | 5     | 2652 | U    |
| 36  | 5     | 2656 | A    |
| 36  | 5     | 2674 | A    |
| 36  | 5     | 2677 | G    |
| 36  | 5     | 2678 | A    |
| 36  | 5     | 2681 | U    |
| 36  | 5     | 2689 | A    |
| 36  | 5     | 2690 | G    |
| 36  | 5     | 2691 | A    |
| 36  | 5     | 2694 | A    |
| 36  | 5     | 2696 | A    |
| 36  | 5     | 2705 | A    |
| 36  | 5     | 2714 | G    |
| 36  | 5     | 2728 | G    |
| 36  | 5     | 2729 | U    |
| 36  | 5     | 2752 | U    |
| 36  | 5     | 2753 | G    |
| 36  | 5     | 2755 | C    |
| 36  | 5     | 2762 | A    |
| 36  | 5     | 2771 | U    |
| 36  | 5     | 2772 | C    |
| 36  | 5     | 2773 | C    |
| 36  | 5     | 2777 | G    |
| 36  | 5     | 2778 | G    |
| 36  | 5     | 2796 | G    |
| 36  | 5     | 2799 | A    |
| 36  | 5     | 2800 | G    |
| 36  | 5     | 2801 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 2810 | C    |
| 36  | 5     | 2817 | A    |
| 36  | 5     | 2818 | U    |
| 36  | 5     | 2819 | A    |
| 36  | 5     | 2822 | U    |
| 36  | 5     | 2843 | U    |
| 36  | 5     | 2845 | A    |
| 36  | 5     | 2853 | A    |
| 36  | 5     | 2871 | G    |
| 36  | 5     | 2872 | A    |
| 36  | 5     | 2874 | G    |
| 36  | 5     | 2875 | U    |
| 36  | 5     | 2887 | A    |
| 36  | 5     | 2888 | U    |
| 36  | 5     | 2896 | A    |
| 36  | 5     | 2897 | A    |
| 36  | 5     | 2899 | C    |
| 36  | 5     | 2902 | A    |
| 36  | 5     | 2923 | U    |
| 36  | 5     | 2935 | U    |
| 36  | 5     | 2936 | A    |
| 36  | 5     | 2942 | C    |
| 36  | 5     | 2945 | G    |
| 36  | 5     | 2947 | G    |
| 36  | 5     | 2971 | A    |
| 36  | 5     | 2972 | G    |
| 36  | 5     | 2979 | U    |
| 36  | 5     | 2983 | C    |
| 36  | 5     | 2990 | G    |
| 36  | 5     | 2992 | U    |
| 36  | 5     | 2996 | U    |
| 36  | 5     | 2997 | G    |
| 36  | 5     | 3006 | A    |
| 36  | 5     | 3012 | A    |
| 36  | 5     | 3033 | A    |
| 36  | 5     | 3049 | A    |
| 36  | 5     | 3050 | U    |
| 36  | 5     | 3056 | U    |
| 36  | 5     | 3057 | U    |
| 36  | 5     | 3059 | G    |
| 36  | 5     | 3078 | U    |
| 36  | 5     | 3079 | U    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 3080 | G    |
| 36  | 5     | 3084 | C    |
| 36  | 5     | 3086 | A    |
| 36  | 5     | 3092 | C    |
| 36  | 5     | 3119 | U    |
| 36  | 5     | 3122 | A    |
| 36  | 5     | 3130 | A    |
| 36  | 5     | 3131 | U    |
| 36  | 5     | 3142 | A    |
| 36  | 5     | 3143 | C    |
| 36  | 5     | 3153 | U    |
| 36  | 5     | 3155 | U    |
| 36  | 5     | 3156 | U    |
| 36  | 5     | 3157 | U    |
| 36  | 5     | 3158 | G    |
| 36  | 5     | 3159 | C    |
| 36  | 5     | 3164 | C    |
| 36  | 5     | 3165 | A    |
| 36  | 5     | 3166 | C    |
| 36  | 5     | 3167 | A    |
| 36  | 5     | 3168 | A    |
| 36  | 5     | 3171 | U    |
| 36  | 5     | 3172 | A    |
| 36  | 5     | 3173 | G    |
| 36  | 5     | 3174 | A    |
| 36  | 5     | 3176 | G    |
| 36  | 5     | 3179 | U    |
| 36  | 5     | 3181 | C    |
| 36  | 5     | 3187 | A    |
| 36  | 5     | 3195 | U    |
| 36  | 5     | 3196 | U    |
| 36  | 5     | 3206 | C    |
| 36  | 5     | 3207 | U    |
| 36  | 5     | 3217 | C    |
| 36  | 5     | 3218 | A    |
| 36  | 5     | 3219 | G    |
| 36  | 5     | 3227 | A    |
| 36  | 5     | 3228 | C    |
| 36  | 5     | 3229 | G    |
| 36  | 5     | 3233 | C    |
| 36  | 5     | 3239 | G    |
| 36  | 5     | 3243 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 3245 | A    |
| 36  | 5     | 3246 | G    |
| 36  | 5     | 3247 | G    |
| 36  | 5     | 3253 | G    |
| 36  | 5     | 3259 | U    |
| 36  | 5     | 3260 | G    |
| 36  | 5     | 3265 | C    |
| 36  | 5     | 3275 | U    |
| 36  | 5     | 3276 | G    |
| 36  | 5     | 3277 | U    |
| 36  | 5     | 3279 | A    |
| 36  | 5     | 3281 | U    |
| 36  | 5     | 3282 | U    |
| 36  | 5     | 3284 | G    |
| 36  | 5     | 3285 | C    |
| 36  | 5     | 3286 | G    |
| 36  | 5     | 3288 | G    |
| 36  | 5     | 3289 | G    |
| 36  | 5     | 3290 | G    |
| 36  | 5     | 3294 | A    |
| 36  | 5     | 3304 | U    |
| 36  | 5     | 3316 | A    |
| 36  | 5     | 3317 | U    |
| 36  | 5     | 3318 | G    |
| 36  | 5     | 3319 | U    |
| 36  | 5     | 3320 | A    |
| 36  | 5     | 3341 | U    |
| 36  | 5     | 3342 | A    |
| 36  | 5     | 3345 | G    |
| 36  | 5     | 3349 | C    |
| 36  | 5     | 3351 | U    |
| 36  | 5     | 3352 | U    |
| 36  | 5     | 3354 | U    |
| 36  | 5     | 3356 | G    |
| 36  | 5     | 3358 | U    |
| 36  | 5     | 3369 | G    |
| 36  | 5     | 3378 | C    |
| 36  | 5     | 3381 | U    |
| 36  | 5     | 3382 | U    |
| 36  | 5     | 3389 | U    |
| 36  | 5     | 3390 | G    |
| 36  | 5     | 3393 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 3396 | U    |
| 37  | 7     | 7    | G    |
| 37  | 7     | 22   | A    |
| 37  | 7     | 33   | U    |
| 37  | 7     | 54   | U    |
| 37  | 7     | 55   | A    |
| 37  | 7     | 60   | G    |
| 37  | 7     | 65   | G    |
| 37  | 7     | 73   | C    |
| 37  | 7     | 76   | A    |
| 37  | 7     | 91   | G    |
| 37  | 7     | 93   | C    |
| 37  | 7     | 102  | A    |
| 37  | 7     | 103  | A    |
| 37  | 7     | 104  | A    |
| 37  | 7     | 112  | G    |
| 38  | 8     | 25   | G    |
| 38  | 8     | 34   | U    |
| 38  | 8     | 35   | C    |
| 38  | 8     | 49   | G    |
| 38  | 8     | 51   | G    |
| 38  | 8     | 52   | A    |
| 38  | 8     | 53   | A    |
| 38  | 8     | 58   | G    |
| 38  | 8     | 59   | A    |
| 38  | 8     | 62   | C    |
| 38  | 8     | 63   | G    |
| 38  | 8     | 79   | A    |
| 38  | 8     | 80   | A    |
| 38  | 8     | 81   | U    |
| 38  | 8     | 82   | U    |
| 38  | 8     | 83   | C    |
| 38  | 8     | 84   | C    |
| 38  | 8     | 86   | U    |
| 38  | 8     | 87   | G    |
| 38  | 8     | 90   | U    |
| 38  | 8     | 95   | G    |
| 38  | 8     | 96   | A    |
| 38  | 8     | 104  | A    |
| 38  | 8     | 105  | A    |
| 38  | 8     | 106  | C    |
| 38  | 8     | 111  | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | 8     | 113 | U    |
| 38  | 8     | 122 | U    |
| 38  | 8     | 125 | U    |
| 38  | 8     | 126 | A    |
| 38  | 8     | 127 | U    |
| 38  | 8     | 138 | A    |
| 38  | 8     | 152 | G    |
| 38  | 8     | 155 | A    |
| 38  | 8     | 156 | U    |
| 38  | 8     | 157 | U    |
| 38  | 8     | 158 | U    |

All (330) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 25  | C    |
| 1   | 2     | 45  | U    |
| 1   | 2     | 68  | A    |
| 1   | 2     | 73  | U    |
| 1   | 2     | 74  | U    |
| 1   | 2     | 93  | A    |
| 1   | 2     | 103 | A    |
| 1   | 2     | 130 | C    |
| 1   | 2     | 131 | C    |
| 1   | 2     | 132 | U    |
| 1   | 2     | 139 | C    |
| 1   | 2     | 144 | U    |
| 1   | 2     | 158 | U    |
| 1   | 2     | 218 | A    |
| 1   | 2     | 240 | U    |
| 1   | 2     | 278 | U    |
| 1   | 2     | 280 | U    |
| 1   | 2     | 352 | A    |
| 1   | 2     | 400 | A    |
| 1   | 2     | 417 | A    |
| 1   | 2     | 468 | A    |
| 1   | 2     | 497 | G    |
| 1   | 2     | 498 | G    |
| 1   | 2     | 499 | U    |
| 1   | 2     | 501 | U    |
| 1   | 2     | 503 | G    |
| 1   | 2     | 510 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 512  | A    |
| 1   | 2     | 558  | U    |
| 1   | 2     | 582  | U    |
| 1   | 2     | 685  | A    |
| 1   | 2     | 704  | C    |
| 1   | 2     | 720  | G    |
| 1   | 2     | 721  | U    |
| 1   | 2     | 734  | A    |
| 1   | 2     | 755  | A    |
| 1   | 2     | 782  | U    |
| 1   | 2     | 794  | U    |
| 1   | 2     | 811  | A    |
| 1   | 2     | 829  | A    |
| 1   | 2     | 1051 | G    |
| 1   | 2     | 1058 | U    |
| 1   | 2     | 1081 | A    |
| 1   | 2     | 1137 | A    |
| 1   | 2     | 1157 | A    |
| 1   | 2     | 1196 | A    |
| 1   | 2     | 1207 | C    |
| 1   | 2     | 1226 | A    |
| 1   | 2     | 1244 | A    |
| 1   | 2     | 1250 | U    |
| 1   | 2     | 1339 | C    |
| 1   | 2     | 1344 | A    |
| 1   | 2     | 1370 | U    |
| 1   | 2     | 1481 | C    |
| 1   | 2     | 1489 | U    |
| 1   | 2     | 1490 | C    |
| 1   | 2     | 1568 | C    |
| 1   | 2     | 1572 | G    |
| 1   | 2     | 1573 | A    |
| 1   | 2     | 1600 | A    |
| 1   | 2     | 1615 | C    |
| 1   | 2     | 1657 | U    |
| 1   | 2     | 1761 | U    |
| 36  | 1     | 43   | A    |
| 36  | 1     | 65   | A    |
| 36  | 1     | 99   | A    |
| 36  | 1     | 169  | U    |
| 36  | 1     | 210  | U    |
| 36  | 1     | 217  | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 223  | U    |
| 36  | 1     | 239  | G    |
| 36  | 1     | 282  | G    |
| 36  | 1     | 397  | A    |
| 36  | 1     | 398  | A    |
| 36  | 1     | 547  | G    |
| 36  | 1     | 588  | G    |
| 36  | 1     | 594  | U    |
| 36  | 1     | 620  | U    |
| 36  | 1     | 637  | C    |
| 36  | 1     | 647  | A    |
| 36  | 1     | 715  | A    |
| 36  | 1     | 719  | U    |
| 36  | 1     | 763  | G    |
| 36  | 1     | 764  | U    |
| 36  | 1     | 816  | A    |
| 36  | 1     | 873  | C    |
| 36  | 1     | 896  | A    |
| 36  | 1     | 916  | G    |
| 36  | 1     | 979  | U    |
| 36  | 1     | 981  | U    |
| 36  | 1     | 993  | G    |
| 36  | 1     | 1064 | A    |
| 36  | 1     | 1094 | U    |
| 36  | 1     | 1097 | G    |
| 36  | 1     | 1103 | A    |
| 36  | 1     | 1196 | C    |
| 36  | 1     | 1273 | A    |
| 36  | 1     | 1307 | G    |
| 36  | 1     | 1317 | A    |
| 36  | 1     | 1329 | U    |
| 36  | 1     | 1352 | A    |
| 36  | 1     | 1355 | A    |
| 36  | 1     | 1481 | A    |
| 36  | 1     | 1484 | U    |
| 36  | 1     | 1507 | G    |
| 36  | 1     | 1514 | G    |
| 36  | 1     | 1554 | U    |
| 36  | 1     | 1562 | C    |
| 36  | 1     | 1607 | U    |
| 36  | 1     | 1643 | A    |
| 36  | 1     | 1716 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 1751 | G    |
| 36  | 1     | 1815 | U    |
| 36  | 1     | 1816 | A    |
| 36  | 1     | 1820 | U    |
| 36  | 1     | 1841 | A    |
| 36  | 1     | 1849 | C    |
| 36  | 1     | 2101 | C    |
| 36  | 1     | 2112 | U    |
| 36  | 1     | 2209 | U    |
| 36  | 1     | 2227 | C    |
| 36  | 1     | 2249 | G    |
| 36  | 1     | 2281 | A    |
| 36  | 1     | 2372 | A    |
| 36  | 1     | 2373 | A    |
| 36  | 1     | 2374 | C    |
| 36  | 1     | 2385 | G    |
| 36  | 1     | 2403 | G    |
| 36  | 1     | 2418 | G    |
| 36  | 1     | 2513 | U    |
| 36  | 1     | 2522 | G    |
| 36  | 1     | 2537 | U    |
| 36  | 1     | 2541 | U    |
| 36  | 1     | 2554 | A    |
| 36  | 1     | 2585 | G    |
| 36  | 1     | 2677 | G    |
| 36  | 1     | 2689 | A    |
| 36  | 1     | 2728 | G    |
| 36  | 1     | 2752 | U    |
| 36  | 1     | 2801 | A    |
| 36  | 1     | 2817 | A    |
| 36  | 1     | 2818 | U    |
| 36  | 1     | 2867 | C    |
| 36  | 1     | 2896 | A    |
| 36  | 1     | 2996 | U    |
| 36  | 1     | 3056 | U    |
| 36  | 1     | 3078 | U    |
| 36  | 1     | 3121 | U    |
| 36  | 1     | 3157 | U    |
| 36  | 1     | 3195 | U    |
| 36  | 1     | 3217 | C    |
| 36  | 1     | 3218 | A    |
| 36  | 1     | 3228 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 1     | 3242 | G    |
| 36  | 1     | 3269 | U    |
| 36  | 1     | 3275 | U    |
| 36  | 1     | 3316 | A    |
| 36  | 1     | 3319 | U    |
| 36  | 1     | 3350 | C    |
| 36  | 1     | 3351 | U    |
| 36  | 1     | 3353 | G    |
| 36  | 1     | 3375 | A    |
| 37  | 3     | 13   | A    |
| 37  | 3     | 49   | G    |
| 38  | 4     | 85   | G    |
| 38  | 4     | 111  | A    |
| 38  | 4     | 125  | U    |
| 1   | 6     | 1    | U    |
| 1   | 6     | 25   | C    |
| 1   | 6     | 66   | U    |
| 1   | 6     | 103  | A    |
| 1   | 6     | 114  | C    |
| 1   | 6     | 136  | C    |
| 1   | 6     | 139  | C    |
| 1   | 6     | 158  | U    |
| 1   | 6     | 187  | G    |
| 1   | 6     | 192  | U    |
| 1   | 6     | 217  | A    |
| 1   | 6     | 240  | U    |
| 1   | 6     | 249  | U    |
| 1   | 6     | 272  | U    |
| 1   | 6     | 277  | U    |
| 1   | 6     | 352  | A    |
| 1   | 6     | 400  | A    |
| 1   | 6     | 417  | A    |
| 1   | 6     | 434  | G    |
| 1   | 6     | 468  | A    |
| 1   | 6     | 512  | A    |
| 1   | 6     | 541  | A    |
| 1   | 6     | 542  | A    |
| 1   | 6     | 557  | G    |
| 1   | 6     | 558  | U    |
| 1   | 6     | 651  | G    |
| 1   | 6     | 667  | U    |
| 1   | 6     | 678  | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 717  | C    |
| 1   | 6     | 755  | A    |
| 1   | 6     | 794  | U    |
| 1   | 6     | 815  | G    |
| 1   | 6     | 829  | A    |
| 1   | 6     | 834  | G    |
| 1   | 6     | 1004 | U    |
| 1   | 6     | 1051 | G    |
| 1   | 6     | 1058 | U    |
| 1   | 6     | 1081 | A    |
| 1   | 6     | 1097 | U    |
| 1   | 6     | 1098 | U    |
| 1   | 6     | 1137 | A    |
| 1   | 6     | 1196 | A    |
| 1   | 6     | 1244 | A    |
| 1   | 6     | 1255 | G    |
| 1   | 6     | 1344 | A    |
| 1   | 6     | 1481 | C    |
| 1   | 6     | 1489 | U    |
| 1   | 6     | 1490 | C    |
| 1   | 6     | 1491 | U    |
| 1   | 6     | 1535 | U    |
| 1   | 6     | 1568 | C    |
| 1   | 6     | 1572 | G    |
| 1   | 6     | 1573 | A    |
| 1   | 6     | 1584 | G    |
| 1   | 6     | 1615 | C    |
| 1   | 6     | 1620 | C    |
| 1   | 6     | 1657 | U    |
| 1   | 6     | 1696 | G    |
| 1   | 6     | 1698 | G    |
| 36  | 5     | 43   | A    |
| 36  | 5     | 65   | A    |
| 36  | 5     | 110  | G    |
| 36  | 5     | 183  | G    |
| 36  | 5     | 210  | U    |
| 36  | 5     | 217  | U    |
| 36  | 5     | 221  | A    |
| 36  | 5     | 238  | A    |
| 36  | 5     | 282  | G    |
| 36  | 5     | 397  | A    |
| 36  | 5     | 588  | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 594  | U    |
| 36  | 5     | 647  | A    |
| 36  | 5     | 715  | A    |
| 36  | 5     | 719  | U    |
| 36  | 5     | 726  | G    |
| 36  | 5     | 735  | A    |
| 36  | 5     | 765  | C    |
| 36  | 5     | 786  | A    |
| 36  | 5     | 816  | A    |
| 36  | 5     | 873  | C    |
| 36  | 5     | 895  | A    |
| 36  | 5     | 896  | A    |
| 36  | 5     | 916  | G    |
| 36  | 5     | 993  | G    |
| 36  | 5     | 1027 | A    |
| 36  | 5     | 1064 | A    |
| 36  | 5     | 1081 | U    |
| 36  | 5     | 1152 | G    |
| 36  | 5     | 1181 | U    |
| 36  | 5     | 1192 | C    |
| 36  | 5     | 1238 | C    |
| 36  | 5     | 1241 | U    |
| 36  | 5     | 1284 | C    |
| 36  | 5     | 1307 | G    |
| 36  | 5     | 1317 | A    |
| 36  | 5     | 1329 | U    |
| 36  | 5     | 1331 | U    |
| 36  | 5     | 1352 | A    |
| 36  | 5     | 1355 | A    |
| 36  | 5     | 1434 | G    |
| 36  | 5     | 1481 | A    |
| 36  | 5     | 1507 | G    |
| 36  | 5     | 1514 | G    |
| 36  | 5     | 1554 | U    |
| 36  | 5     | 1560 | G    |
| 36  | 5     | 1589 | A    |
| 36  | 5     | 1716 | U    |
| 36  | 5     | 1725 | C    |
| 36  | 5     | 1815 | U    |
| 36  | 5     | 1816 | A    |
| 36  | 5     | 1841 | A    |
| 36  | 5     | 1846 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1849 | C    |
| 36  | 5     | 2101 | C    |
| 36  | 5     | 2112 | U    |
| 36  | 5     | 2116 | G    |
| 36  | 5     | 2204 | C    |
| 36  | 5     | 2209 | U    |
| 36  | 5     | 2249 | G    |
| 36  | 5     | 2255 | A    |
| 36  | 5     | 2256 | A    |
| 36  | 5     | 2257 | C    |
| 36  | 5     | 2372 | A    |
| 36  | 5     | 2373 | A    |
| 36  | 5     | 2374 | C    |
| 36  | 5     | 2385 | G    |
| 36  | 5     | 2398 | A    |
| 36  | 5     | 2440 | G    |
| 36  | 5     | 2507 | C    |
| 36  | 5     | 2513 | U    |
| 36  | 5     | 2531 | C    |
| 36  | 5     | 2539 | C    |
| 36  | 5     | 2584 | G    |
| 36  | 5     | 2585 | G    |
| 36  | 5     | 2593 | A    |
| 36  | 5     | 2704 | A    |
| 36  | 5     | 2728 | G    |
| 36  | 5     | 2772 | C    |
| 36  | 5     | 2801 | A    |
| 36  | 5     | 2817 | A    |
| 36  | 5     | 2818 | U    |
| 36  | 5     | 2887 | A    |
| 36  | 5     | 2896 | A    |
| 36  | 5     | 2971 | A    |
| 36  | 5     | 3049 | A    |
| 36  | 5     | 3056 | U    |
| 36  | 5     | 3078 | U    |
| 36  | 5     | 3121 | U    |
| 36  | 5     | 3154 | C    |
| 36  | 5     | 3195 | U    |
| 36  | 5     | 3218 | A    |
| 36  | 5     | 3228 | C    |
| 36  | 5     | 3242 | G    |
| 36  | 5     | 3259 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 3275 | U    |
| 36  | 5     | 3289 | G    |
| 36  | 5     | 3317 | U    |
| 36  | 5     | 3340 | G    |
| 36  | 5     | 3341 | U    |
| 36  | 5     | 3357 | U    |
| 37  | 7     | 49   | G    |
| 38  | 8     | 59   | A    |
| 38  | 8     | 111  | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 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 | $\# Z  > 2$ |
| 86  | OHX  | C5    | 201  | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3904 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 14    | 403  | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4105 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2170 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4124 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2171 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2112 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4237 | -    | 0,6,6        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3937 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M6    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m1    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3870 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4158 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 4     | 234  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4208 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4236 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s9    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4228 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l3    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 229  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O2    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3958 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3883 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3967 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2073 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4216 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3951 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3920 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m0    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4218 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3971 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 8     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3878 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 230  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3998 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3888 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3937 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4224 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3967 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3924 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 215  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s1    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3904 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | N9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l3    | 404  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3900 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O7    | 103  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3892 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3948 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4250 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4238 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 229  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4053 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3968 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2192 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3869 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 215  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s8    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3975 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3899 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L3    | 404  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4131 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4241 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | 3H3  | 5     | 4251 | -    | 34,34,34     | 1.04 | 2 (5%)   | 36,45,45    | 1.45 | 4 (11%)  |
| 86  | OHX  | 1     | 4008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3961 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3948 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3991 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3954 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3931 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4226 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4242 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3966 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3928 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 228  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m5    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4210 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3900 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4243 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4244 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m4    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M0    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3911 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3920 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2078 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4248 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3891 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3897 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4235 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3893 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2147 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 19    | 600  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3881 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | 3H3  | 1     | 4216 | -    | 34,34,34     | 1.09 | 3 (8%)   | 36,45,45    | 2.02 | 8 (22%)  |
| 86  | OHX  | 5     | 4213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3968 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4207 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | d9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3875 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 233  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3899 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 236  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4192 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3939 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4160 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4227 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3990 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3966 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3898 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4225 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3885 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | SR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | q2    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4210 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3880 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4116 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3887 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O3    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4223 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3991 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3963 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3983 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4027 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3890 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3879 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4245 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3998 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4207 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3923 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3868 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | n3    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2066 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M5    | 304  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4222 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3931 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3884 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3911 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2152 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4221 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3939 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3877 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4246 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3898 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3873 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3923 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 4202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2032 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4231 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o2    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | D9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3917 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4192 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 232  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3961 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2124 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o4    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l5    | 305  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3942 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m6    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3917 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3918 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s4    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3876 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M7    | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o3    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | S8    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3942 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l5    | 306  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M5    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4151 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 4081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o7    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3928 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3886 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4247 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3983 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 214  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 14    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3894 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3954 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m7    | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4163 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4240 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4232 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4220 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4234 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4229 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3963 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2156 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3945 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C3    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4233 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4214 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3924 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | Q2    | 503  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3919 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3990 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L6    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 4004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M7    | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m0    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | sR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 231  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3918 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4208 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3958 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L4    | 404  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3945 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C1    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4249 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s1    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 228  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4105 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L3    | 403  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3882 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c8    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 235  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3889 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4172 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4230 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M9    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3951 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l3    | 403  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4219 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3975 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4214 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4239 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3919 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4133 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3871 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | d4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3874 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c1    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | n9    | 3803 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4217 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3896 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O7    | 104  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3895 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4073 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3872 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3971 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 15    | 304  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4075 | -    | 0,6,6        | -    | -        | -           |      |          |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 88  | 3H3  | 1     | 4216 | -    | -       | 8/39/51/51 | 0/1/2/2 |
| 88  | 3H3  | 5     | 4251 | -    | -       | 8/39/51/51 | 0/1/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 88  | 1     | 4216 | 3H3  | C3-C2   | 3.85  | 1.47        | 1.33     |
| 88  | 5     | 4251 | 3H3  | C14-C16 | 3.70  | 1.56        | 1.53     |
| 88  | 5     | 4251 | 3H3  | C15-C14 | -3.01 | 1.50        | 1.54     |
| 88  | 1     | 4216 | 3H3  | C15-C14 | -3.01 | 1.50        | 1.54     |
| 88  | 1     | 4216 | 3H3  | C14-C13 | 2.33  | 1.54        | 1.50     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 88  | 1     | 4216 | 3H3  | C-C1-C11    | 6.38  | 119.56      | 110.78   |
| 88  | 1     | 4216 | 3H3  | C1-C11-C12  | 5.18  | 122.64      | 113.19   |
| 88  | 5     | 4251 | 3H3  | C15-C14-C16 | 4.98  | 116.50      | 109.31   |
| 88  | 1     | 4216 | 3H3  | C15-C14-C16 | 4.94  | 116.44      | 109.31   |
| 88  | 5     | 4251 | 3H3  | C1-C11-C12  | 4.10  | 120.67      | 113.19   |
| 88  | 1     | 4216 | 3H3  | C-C1-C2     | -3.49 | 102.02      | 109.91   |
| 88  | 1     | 4216 | 3H3  | O1-C11-C12  | -2.90 | 103.55      | 110.19   |
| 88  | 1     | 4216 | 3H3  | C6-C7-C8    | -2.29 | 106.97      | 112.73   |
| 88  | 1     | 4216 | 3H3  | C8-C9-C10   | -2.22 | 117.49      | 122.78   |
| 88  | 5     | 4251 | 3H3  | C6-C7-C8    | -2.16 | 107.32      | 112.73   |
| 88  | 5     | 4251 | 3H3  | O2-C16-C17  | 2.11  | 124.38      | 121.40   |
| 88  | 1     | 4216 | 3H3  | O2-C16-C17  | 2.05  | 124.30      | 121.40   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 88  | 1     | 4216 | 3H3  | C2-C1-C11-O1    |
| 88  | 1     | 4216 | 3H3  | C2-C1-C11-C12   |
| 88  | 1     | 4216 | 3H3  | C-C1-C11-O1     |
| 88  | 1     | 4216 | 3H3  | C-C1-C11-C12    |
| 88  | 5     | 4251 | 3H3  | C12-C11-O1-C10  |
| 88  | 5     | 4251 | 3H3  | C1-C11-O1-C10   |
| 88  | 5     | 4251 | 3H3  | C1-C2-C3-C4     |
| 88  | 5     | 4251 | 3H3  | C9-C10-O1-C11   |
| 88  | 1     | 4216 | 3H3  | C2-C3-C4-C5     |
| 88  | 5     | 4251 | 3H3  | O-C10-O1-C11    |
| 88  | 5     | 4251 | 3H3  | C2-C3-C4-C5     |
| 88  | 5     | 4251 | 3H3  | C6-C7-C8-C9     |
| 88  | 1     | 4216 | 3H3  | C12-C13-C14-C16 |
| 88  | 1     | 4216 | 3H3  | C13-C14-C16-O2  |
| 88  | 5     | 4251 | 3H3  | C13-C14-C16-O2  |
| 88  | 1     | 4216 | 3H3  | C6-C7-C8-C9     |

There are no ring outliers.

481 monomers are involved in 810 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | C5    | 201  | OHX  | 2       | 0            |
| 86  | 2     | 2170 | OHX  | 1       | 0            |
| 86  | 6     | 2171 | OHX  | 8       | 0            |
| 86  | 5     | 4003 | OHX  | 1       | 0            |
| 86  | 6     | 2138 | OHX  | 1       | 0            |
| 86  | 1     | 3937 | OHX  | 1       | 0            |
| 86  | 2     | 2163 | OHX  | 6       | 0            |
| 86  | M6    | 202  | OHX  | 1       | 0            |
| 86  | 5     | 4182 | OHX  | 1       | 0            |
| 86  | 5     | 4076 | OHX  | 4       | 0            |
| 86  | 6     | 2136 | OHX  | 1       | 0            |
| 86  | 5     | 4001 | OHX  | 7       | 0            |
| 86  | 5     | 4193 | OHX  | 1       | 0            |
| 86  | 6     | 2157 | OHX  | 1       | 0            |
| 86  | m1    | 203  | OHX  | 1       | 0            |
| 86  | 6     | 2103 | OHX  | 2       | 0            |
| 86  | 1     | 4054 | OHX  | 1       | 0            |
| 86  | 1     | 4182 | OHX  | 1       | 0            |
| 86  | 1     | 4012 | OHX  | 1       | 0            |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 5     | 4089 | OHX  | 1       | 0            |
| 86  | 1     | 3935 | OHX  | 2       | 0            |
| 86  | 1     | 4158 | OHX  | 4       | 0            |
| 86  | 6     | 2062 | OHX  | 1       | 0            |
| 86  | 1     | 4138 | OHX  | 3       | 0            |
| 86  | 5     | 4205 | OHX  | 1       | 0            |
| 86  | 1     | 4208 | OHX  | 1       | 0            |
| 86  | 1     | 4034 | OHX  | 2       | 0            |
| 86  | 1     | 4171 | OHX  | 1       | 0            |
| 86  | 2     | 2043 | OHX  | 1       | 0            |
| 86  | s9    | 201  | OHX  | 2       | 0            |
| 86  | 5     | 4191 | OHX  | 1       | 0            |
| 86  | 2     | 2150 | OHX  | 1       | 0            |
| 86  | 1     | 4167 | OHX  | 2       | 0            |
| 86  | 1     | 3943 | OHX  | 6       | 0            |
| 86  | 2     | 2037 | OHX  | 3       | 0            |
| 86  | 5     | 4066 | OHX  | 7       | 0            |
| 86  | 1     | 3970 | OHX  | 1       | 0            |
| 86  | 2     | 2072 | OHX  | 1       | 0            |
| 86  | 1     | 3883 | OHX  | 1       | 0            |
| 86  | 2     | 2049 | OHX  | 1       | 0            |
| 86  | 5     | 3972 | OHX  | 1       | 0            |
| 86  | 6     | 2073 | OHX  | 1       | 0            |
| 86  | 1     | 4068 | OHX  | 1       | 0            |
| 86  | 7     | 224  | OHX  | 4       | 0            |
| 86  | 2     | 2086 | OHX  | 4       | 0            |
| 86  | 6     | 2149 | OHX  | 1       | 0            |
| 86  | 2     | 2133 | OHX  | 1       | 0            |
| 86  | 6     | 2060 | OHX  | 6       | 0            |
| 86  | 1     | 4005 | OHX  | 1       | 0            |
| 86  | 1     | 4047 | OHX  | 4       | 0            |
| 86  | 2     | 2167 | OHX  | 2       | 0            |
| 86  | 5     | 4013 | OHX  | 2       | 0            |
| 86  | 2     | 2073 | OHX  | 1       | 0            |
| 86  | 2     | 2160 | OHX  | 2       | 0            |
| 86  | m0    | 301  | OHX  | 1       | 0            |
| 86  | 6     | 2163 | OHX  | 1       | 0            |
| 86  | 7     | 219  | OHX  | 4       | 0            |
| 86  | 1     | 3971 | OHX  | 1       | 0            |
| 86  | 2     | 2065 | OHX  | 1       | 0            |
| 86  | 5     | 4185 | OHX  | 1       | 0            |
| 86  | 2     | 2074 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 5     | 4118 | OHX  | 1       | 0            |
| 86  | 2     | 2121 | OHX  | 2       | 0            |
| 86  | 1     | 3888 | OHX  | 1       | 0            |
| 86  | 1     | 4102 | OHX  | 1       | 0            |
| 86  | 1     | 4147 | OHX  | 1       | 0            |
| 86  | 5     | 4224 | OHX  | 2       | 0            |
| 86  | 1     | 4041 | OHX  | 3       | 0            |
| 86  | 6     | 2066 | OHX  | 1       | 0            |
| 86  | 1     | 4066 | OHX  | 1       | 0            |
| 86  | 5     | 4128 | OHX  | 1       | 0            |
| 86  | 8     | 219  | OHX  | 2       | 0            |
| 86  | 1     | 4095 | OHX  | 1       | 0            |
| 86  | 6     | 2175 | OHX  | 1       | 0            |
| 86  | 1     | 3967 | OHX  | 1       | 0            |
| 86  | 1     | 3987 | OHX  | 2       | 0            |
| 86  | 5     | 3924 | OHX  | 3       | 0            |
| 86  | 2     | 2130 | OHX  | 2       | 0            |
| 86  | 2     | 2117 | OHX  | 1       | 0            |
| 86  | 6     | 2154 | OHX  | 2       | 0            |
| 86  | 1     | 4023 | OHX  | 7       | 0            |
| 86  | 5     | 4145 | OHX  | 1       | 0            |
| 86  | 1     | 4203 | OHX  | 1       | 0            |
| 86  | 2     | 2071 | OHX  | 1       | 0            |
| 86  | 6     | 2074 | OHX  | 2       | 0            |
| 86  | 6     | 2150 | OHX  | 5       | 0            |
| 86  | 6     | 2143 | OHX  | 1       | 0            |
| 86  | 5     | 4196 | OHX  | 9       | 0            |
| 86  | 5     | 4051 | OHX  | 1       | 0            |
| 86  | 1     | 4049 | OHX  | 1       | 0            |
| 86  | 1     | 4153 | OHX  | 7       | 0            |
| 86  | 5     | 4072 | OHX  | 1       | 0            |
| 86  | 5     | 4039 | OHX  | 1       | 0            |
| 86  | 5     | 3904 | OHX  | 1       | 0            |
| 86  | N9    | 101  | OHX  | 1       | 0            |
| 86  | 1     | 4094 | OHX  | 1       | 0            |
| 86  | 5     | 4183 | OHX  | 1       | 0            |
| 86  | 1     | 4064 | OHX  | 1       | 0            |
| 86  | O7    | 103  | OHX  | 7       | 0            |
| 86  | 1     | 3976 | OHX  | 7       | 0            |
| 86  | 1     | 4187 | OHX  | 1       | 0            |
| 86  | 1     | 3979 | OHX  | 1       | 0            |
| 86  | 2     | 2109 | OHX  | 7       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 6     | 2188 | OHX  | 1       | 0            |
| 86  | 5     | 3948 | OHX  | 1       | 0            |
| 86  | 5     | 4144 | OHX  | 1       | 0            |
| 86  | 1     | 4166 | OHX  | 6       | 0            |
| 86  | 5     | 4026 | OHX  | 1       | 0            |
| 86  | 5     | 3912 | OHX  | 1       | 0            |
| 86  | 2     | 2155 | OHX  | 4       | 0            |
| 86  | 5     | 4238 | OHX  | 2       | 0            |
| 86  | 3     | 218  | OHX  | 3       | 0            |
| 86  | 2     | 2172 | OHX  | 2       | 0            |
| 86  | 6     | 2096 | OHX  | 1       | 0            |
| 86  | 5     | 4002 | OHX  | 2       | 0            |
| 86  | 2     | 2142 | OHX  | 1       | 0            |
| 86  | 1     | 4048 | OHX  | 7       | 0            |
| 86  | 2     | 2077 | OHX  | 1       | 0            |
| 86  | 5     | 4161 | OHX  | 1       | 0            |
| 86  | 1     | 4134 | OHX  | 1       | 0            |
| 86  | 5     | 4109 | OHX  | 1       | 0            |
| 86  | 1     | 3968 | OHX  | 3       | 0            |
| 86  | 1     | 4038 | OHX  | 1       | 0            |
| 86  | 6     | 2192 | OHX  | 1       | 0            |
| 86  | 5     | 4176 | OHX  | 1       | 0            |
| 86  | 6     | 2094 | OHX  | 1       | 0            |
| 86  | 7     | 226  | OHX  | 6       | 0            |
| 86  | 2     | 2157 | OHX  | 1       | 0            |
| 86  | 1     | 4032 | OHX  | 6       | 0            |
| 86  | 8     | 215  | OHX  | 6       | 0            |
| 86  | 6     | 2115 | OHX  | 2       | 0            |
| 86  | 6     | 2155 | OHX  | 1       | 0            |
| 86  | 5     | 4024 | OHX  | 2       | 0            |
| 86  | 1     | 4043 | OHX  | 2       | 0            |
| 86  | 5     | 4108 | OHX  | 3       | 0            |
| 86  | s8    | 303  | OHX  | 1       | 0            |
| 86  | 1     | 4014 | OHX  | 1       | 0            |
| 86  | 2     | 2119 | OHX  | 1       | 0            |
| 86  | 5     | 4141 | OHX  | 6       | 0            |
| 86  | 6     | 2142 | OHX  | 1       | 0            |
| 86  | 7     | 221  | OHX  | 1       | 0            |
| 86  | 1     | 4183 | OHX  | 1       | 0            |
| 86  | 6     | 2097 | OHX  | 1       | 0            |
| 86  | 6     | 2113 | OHX  | 1       | 0            |
| 86  | 5     | 4131 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 5     | 4241 | OHX  | 7       | 0            |
| 88  | 5     | 4251 | 3H3  | 1       | 0            |
| 86  | 2     | 2105 | OHX  | 1       | 0            |
| 86  | 1     | 3952 | OHX  | 1       | 0            |
| 86  | 6     | 2055 | OHX  | 1       | 0            |
| 86  | 5     | 4127 | OHX  | 1       | 0            |
| 86  | 5     | 4215 | OHX  | 8       | 0            |
| 86  | 1     | 3948 | OHX  | 1       | 0            |
| 86  | 6     | 2160 | OHX  | 1       | 0            |
| 86  | 5     | 4102 | OHX  | 2       | 0            |
| 86  | 5     | 4226 | OHX  | 1       | 0            |
| 86  | 5     | 4242 | OHX  | 1       | 0            |
| 86  | 1     | 4056 | OHX  | 6       | 0            |
| 86  | 1     | 4151 | OHX  | 1       | 0            |
| 86  | 5     | 3987 | OHX  | 1       | 0            |
| 86  | 5     | 4177 | OHX  | 2       | 0            |
| 86  | 6     | 2093 | OHX  | 1       | 0            |
| 86  | 6     | 2089 | OHX  | 1       | 0            |
| 86  | O9    | 101  | OHX  | 4       | 0            |
| 86  | 1     | 4210 | OHX  | 1       | 0            |
| 86  | 6     | 2196 | OHX  | 1       | 0            |
| 86  | 8     | 218  | OHX  | 1       | 0            |
| 86  | 1     | 4122 | OHX  | 2       | 0            |
| 86  | 1     | 4113 | OHX  | 1       | 0            |
| 86  | 2     | 2158 | OHX  | 3       | 0            |
| 86  | 6     | 2061 | OHX  | 1       | 0            |
| 86  | 5     | 3973 | OHX  | 6       | 0            |
| 86  | 5     | 4132 | OHX  | 1       | 0            |
| 86  | 5     | 4187 | OHX  | 7       | 0            |
| 86  | 5     | 4181 | OHX  | 1       | 0            |
| 86  | 5     | 4212 | OHX  | 6       | 0            |
| 86  | 5     | 4179 | OHX  | 1       | 0            |
| 86  | 1     | 3897 | OHX  | 1       | 0            |
| 86  | 5     | 4097 | OHX  | 1       | 0            |
| 86  | 2     | 2090 | OHX  | 6       | 0            |
| 86  | 1     | 4021 | OHX  | 1       | 0            |
| 86  | 5     | 4235 | OHX  | 1       | 0            |
| 86  | 8     | 224  | OHX  | 6       | 0            |
| 86  | 5     | 4130 | OHX  | 1       | 0            |
| 86  | 1     | 4061 | OHX  | 5       | 0            |
| 86  | 1     | 4083 | OHX  | 1       | 0            |
| 86  | 5     | 4033 | OHX  | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 2     | 2147 | OHX  | 7       | 0            |
| 86  | 1     | 4177 | OHX  | 6       | 0            |
| 88  | 1     | 4216 | 3H3  | 1       | 0            |
| 86  | 1     | 3903 | OHX  | 1       | 0            |
| 86  | 5     | 4094 | OHX  | 6       | 0            |
| 86  | d9    | 102  | OHX  | 1       | 0            |
| 86  | 5     | 4200 | OHX  | 1       | 0            |
| 86  | 5     | 4206 | OHX  | 1       | 0            |
| 86  | 1     | 3875 | OHX  | 1       | 0            |
| 86  | 2     | 2127 | OHX  | 1       | 0            |
| 86  | 5     | 4157 | OHX  | 2       | 0            |
| 86  | 2     | 2168 | OHX  | 1       | 0            |
| 86  | 1     | 4059 | OHX  | 7       | 0            |
| 86  | 5     | 4020 | OHX  | 6       | 0            |
| 86  | 1     | 4071 | OHX  | 6       | 0            |
| 86  | 5     | 3941 | OHX  | 1       | 0            |
| 86  | 2     | 2166 | OHX  | 1       | 0            |
| 86  | 1     | 4135 | OHX  | 3       | 0            |
| 86  | 2     | 2116 | OHX  | 7       | 0            |
| 86  | 5     | 4096 | OHX  | 1       | 0            |
| 86  | 1     | 4046 | OHX  | 2       | 0            |
| 86  | 6     | 2144 | OHX  | 1       | 0            |
| 86  | 1     | 4201 | OHX  | 1       | 0            |
| 86  | 5     | 4160 | OHX  | 2       | 0            |
| 86  | 5     | 4227 | OHX  | 1       | 0            |
| 86  | 2     | 2173 | OHX  | 2       | 0            |
| 86  | 6     | 2075 | OHX  | 2       | 0            |
| 86  | 6     | 2183 | OHX  | 1       | 0            |
| 86  | 8     | 225  | OHX  | 1       | 0            |
| 86  | 1     | 3990 | OHX  | 1       | 0            |
| 86  | 5     | 3953 | OHX  | 1       | 0            |
| 86  | 6     | 2168 | OHX  | 1       | 0            |
| 86  | 5     | 3966 | OHX  | 1       | 0            |
| 86  | 6     | 2067 | OHX  | 1       | 0            |
| 86  | 1     | 4099 | OHX  | 1       | 0            |
| 86  | C8    | 201  | OHX  | 1       | 0            |
| 86  | 1     | 3898 | OHX  | 1       | 0            |
| 86  | 5     | 4225 | OHX  | 1       | 0            |
| 86  | 2     | 2096 | OHX  | 6       | 0            |
| 86  | 3     | 216  | OHX  | 1       | 0            |
| 86  | q2    | 502  | OHX  | 3       | 0            |
| 86  | 5     | 3921 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 1     | 3887 | OHX  | 1       | 0            |
| 86  | 5     | 3969 | OHX  | 1       | 0            |
| 86  | 1     | 4168 | OHX  | 1       | 0            |
| 86  | 5     | 4088 | OHX  | 1       | 0            |
| 86  | 6     | 2147 | OHX  | 7       | 0            |
| 86  | 2     | 2094 | OHX  | 1       | 0            |
| 86  | 1     | 4200 | OHX  | 6       | 0            |
| 86  | 2     | 2110 | OHX  | 1       | 0            |
| 86  | 5     | 3957 | OHX  | 1       | 0            |
| 86  | 5     | 4106 | OHX  | 1       | 0            |
| 86  | 1     | 4157 | OHX  | 5       | 0            |
| 86  | 5     | 3991 | OHX  | 2       | 0            |
| 86  | 1     | 3980 | OHX  | 5       | 0            |
| 86  | 1     | 4079 | OHX  | 1       | 0            |
| 86  | 1     | 3983 | OHX  | 1       | 0            |
| 86  | 2     | 2097 | OHX  | 1       | 0            |
| 86  | 5     | 4129 | OHX  | 1       | 0            |
| 86  | 1     | 4042 | OHX  | 1       | 0            |
| 86  | 5     | 3949 | OHX  | 1       | 0            |
| 86  | 5     | 4207 | OHX  | 2       | 0            |
| 86  | 2     | 2027 | OHX  | 2       | 0            |
| 86  | 2     | 2174 | OHX  | 1       | 0            |
| 86  | 5     | 4138 | OHX  | 1       | 0            |
| 86  | 1     | 4017 | OHX  | 1       | 0            |
| 86  | 5     | 3978 | OHX  | 8       | 0            |
| 86  | 1     | 4070 | OHX  | 1       | 0            |
| 86  | 1     | 4118 | OHX  | 6       | 0            |
| 86  | M5    | 304  | OHX  | 1       | 0            |
| 86  | 6     | 2102 | OHX  | 1       | 0            |
| 86  | 5     | 4110 | OHX  | 1       | 0            |
| 86  | 2     | 2137 | OHX  | 1       | 0            |
| 86  | 8     | 222  | OHX  | 2       | 0            |
| 86  | 2     | 2045 | OHX  | 6       | 0            |
| 86  | 2     | 2131 | OHX  | 1       | 0            |
| 86  | 5     | 4017 | OHX  | 1       | 0            |
| 86  | 1     | 4179 | OHX  | 1       | 0            |
| 86  | 1     | 4010 | OHX  | 1       | 0            |
| 86  | 5     | 4166 | OHX  | 1       | 0            |
| 86  | 5     | 4222 | OHX  | 6       | 0            |
| 86  | 1     | 3931 | OHX  | 1       | 0            |
| 86  | 1     | 3911 | OHX  | 1       | 0            |
| 86  | 1     | 4123 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 6     | 2108 | OHX  | 1       | 0            |
| 86  | 1     | 3973 | OHX  | 1       | 0            |
| 86  | 1     | 4016 | OHX  | 1       | 0            |
| 86  | 5     | 4221 | OHX  | 1       | 0            |
| 86  | 6     | 2135 | OHX  | 1       | 0            |
| 86  | 6     | 2180 | OHX  | 1       | 0            |
| 86  | 6     | 2202 | OHX  | 2       | 0            |
| 86  | 1     | 4044 | OHX  | 2       | 0            |
| 86  | 1     | 3962 | OHX  | 5       | 0            |
| 86  | 5     | 4007 | OHX  | 1       | 0            |
| 86  | 5     | 4198 | OHX  | 7       | 0            |
| 86  | 5     | 4117 | OHX  | 3       | 0            |
| 86  | 1     | 4088 | OHX  | 7       | 0            |
| 86  | 1     | 4186 | OHX  | 1       | 0            |
| 86  | 2     | 2085 | OHX  | 1       | 0            |
| 86  | 6     | 2123 | OHX  | 1       | 0            |
| 86  | 5     | 3955 | OHX  | 2       | 0            |
| 86  | 5     | 4090 | OHX  | 7       | 0            |
| 86  | 5     | 4189 | OHX  | 7       | 0            |
| 86  | 4     | 227  | OHX  | 1       | 0            |
| 86  | 1     | 4136 | OHX  | 3       | 0            |
| 86  | 5     | 4204 | OHX  | 1       | 0            |
| 86  | 1     | 3873 | OHX  | 1       | 0            |
| 86  | 2     | 2039 | OHX  | 1       | 0            |
| 86  | 4     | 224  | OHX  | 1       | 0            |
| 86  | 5     | 4093 | OHX  | 4       | 0            |
| 86  | 2     | 2145 | OHX  | 1       | 0            |
| 86  | 5     | 4074 | OHX  | 5       | 0            |
| 86  | 8     | 216  | OHX  | 1       | 0            |
| 86  | 2     | 2032 | OHX  | 7       | 0            |
| 86  | 2     | 2162 | OHX  | 1       | 0            |
| 86  | 1     | 4170 | OHX  | 2       | 0            |
| 86  | 5     | 4054 | OHX  | 3       | 0            |
| 86  | 2     | 2115 | OHX  | 2       | 0            |
| 86  | 1     | 4149 | OHX  | 6       | 0            |
| 86  | 2     | 2161 | OHX  | 2       | 0            |
| 86  | 4     | 232  | OHX  | 2       | 0            |
| 86  | 5     | 4068 | OHX  | 1       | 0            |
| 86  | 2     | 2169 | OHX  | 1       | 0            |
| 86  | 1     | 3961 | OHX  | 1       | 0            |
| 86  | 6     | 2124 | OHX  | 1       | 0            |
| 86  | 1     | 4084 | OHX  | 8       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 1     | 3993 | OHX  | 1       | 0            |
| 86  | 2     | 2128 | OHX  | 1       | 0            |
| 86  | 5     | 4046 | OHX  | 1       | 0            |
| 86  | o4    | 203  | OHX  | 4       | 0            |
| 86  | 6     | 2101 | OHX  | 3       | 0            |
| 86  | 1     | 4051 | OHX  | 2       | 0            |
| 86  | l5    | 305  | OHX  | 1       | 0            |
| 86  | 5     | 3942 | OHX  | 3       | 0            |
| 86  | 5     | 4030 | OHX  | 1       | 0            |
| 86  | 2     | 2075 | OHX  | 1       | 0            |
| 86  | 2     | 2040 | OHX  | 2       | 0            |
| 86  | 6     | 2178 | OHX  | 1       | 0            |
| 86  | 1     | 4092 | OHX  | 1       | 0            |
| 86  | 5     | 4119 | OHX  | 1       | 0            |
| 86  | s4    | 301  | OHX  | 1       | 0            |
| 86  | 2     | 2144 | OHX  | 1       | 0            |
| 86  | 1     | 3876 | OHX  | 1       | 0            |
| 86  | 5     | 4034 | OHX  | 4       | 0            |
| 86  | S8    | 302  | OHX  | 1       | 0            |
| 86  | 1     | 4159 | OHX  | 6       | 0            |
| 86  | 5     | 4146 | OHX  | 1       | 0            |
| 86  | M5    | 303  | OHX  | 1       | 0            |
| 86  | 5     | 4151 | OHX  | 1       | 0            |
| 86  | 1     | 4146 | OHX  | 2       | 0            |
| 86  | o7    | 502  | OHX  | 1       | 0            |
| 86  | 1     | 4175 | OHX  | 8       | 0            |
| 86  | 5     | 4065 | OHX  | 5       | 0            |
| 86  | 5     | 4140 | OHX  | 2       | 0            |
| 86  | 1     | 3886 | OHX  | 1       | 0            |
| 86  | 6     | 2120 | OHX  | 2       | 0            |
| 86  | 1     | 3985 | OHX  | 1       | 0            |
| 86  | 5     | 4247 | OHX  | 2       | 0            |
| 86  | 6     | 2162 | OHX  | 1       | 0            |
| 86  | 2     | 2052 | OHX  | 1       | 0            |
| 86  | 8     | 214  | OHX  | 2       | 0            |
| 86  | 1     | 4077 | OHX  | 1       | 0            |
| 86  | 6     | 2170 | OHX  | 1       | 0            |
| 86  | l4    | 402  | OHX  | 3       | 0            |
| 86  | 1     | 4076 | OHX  | 3       | 0            |
| 86  | 6     | 2118 | OHX  | 1       | 0            |
| 86  | 1     | 4209 | OHX  | 1       | 0            |
| 86  | 2     | 2076 | OHX  | 6       | 0            |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 1     | 4100 | OHX  | 1       | 0            |
| 86  | 6     | 2107 | OHX  | 1       | 0            |
| 86  | 6     | 2130 | OHX  | 1       | 0            |
| 86  | 7     | 217  | OHX  | 1       | 0            |
| 86  | 1     | 4036 | OHX  | 6       | 0            |
| 86  | 2     | 2083 | OHX  | 1       | 0            |
| 86  | 5     | 3962 | OHX  | 4       | 0            |
| 86  | 2     | 2091 | OHX  | 6       | 0            |
| 86  | 3     | 226  | OHX  | 1       | 0            |
| 86  | 6     | 2112 | OHX  | 1       | 0            |
| 86  | 6     | 2190 | OHX  | 2       | 0            |
| 86  | 5     | 3959 | OHX  | 1       | 0            |
| 86  | m7    | 206  | OHX  | 1       | 0            |
| 86  | 5     | 4170 | OHX  | 1       | 0            |
| 86  | 1     | 4163 | OHX  | 5       | 0            |
| 86  | 2     | 2059 | OHX  | 1       | 0            |
| 86  | 5     | 4011 | OHX  | 6       | 0            |
| 86  | 5     | 4232 | OHX  | 2       | 0            |
| 86  | 2     | 2111 | OHX  | 2       | 0            |
| 86  | 1     | 4060 | OHX  | 4       | 0            |
| 86  | 2     | 2058 | OHX  | 1       | 0            |
| 86  | 5     | 4079 | OHX  | 1       | 0            |
| 86  | 2     | 2132 | OHX  | 8       | 0            |
| 86  | 5     | 4234 | OHX  | 6       | 0            |
| 86  | 3     | 223  | OHX  | 2       | 0            |
| 86  | 5     | 4203 | OHX  | 1       | 0            |
| 86  | 5     | 4136 | OHX  | 2       | 0            |
| 86  | 1     | 4007 | OHX  | 8       | 0            |
| 86  | 1     | 4011 | OHX  | 1       | 0            |
| 86  | 6     | 2159 | OHX  | 3       | 0            |
| 86  | 5     | 4197 | OHX  | 7       | 0            |
| 86  | 1     | 4205 | OHX  | 2       | 0            |
| 86  | 2     | 2156 | OHX  | 1       | 0            |
| 86  | 2     | 2139 | OHX  | 1       | 0            |
| 86  | 2     | 2084 | OHX  | 4       | 0            |
| 86  | 5     | 4000 | OHX  | 5       | 0            |
| 86  | 6     | 2126 | OHX  | 3       | 0            |
| 86  | 5     | 4091 | OHX  | 1       | 0            |
| 86  | 1     | 4111 | OHX  | 1       | 0            |
| 86  | 6     | 2189 | OHX  | 2       | 0            |
| 86  | 5     | 4201 | OHX  | 5       | 0            |
| 86  | 1     | 3945 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

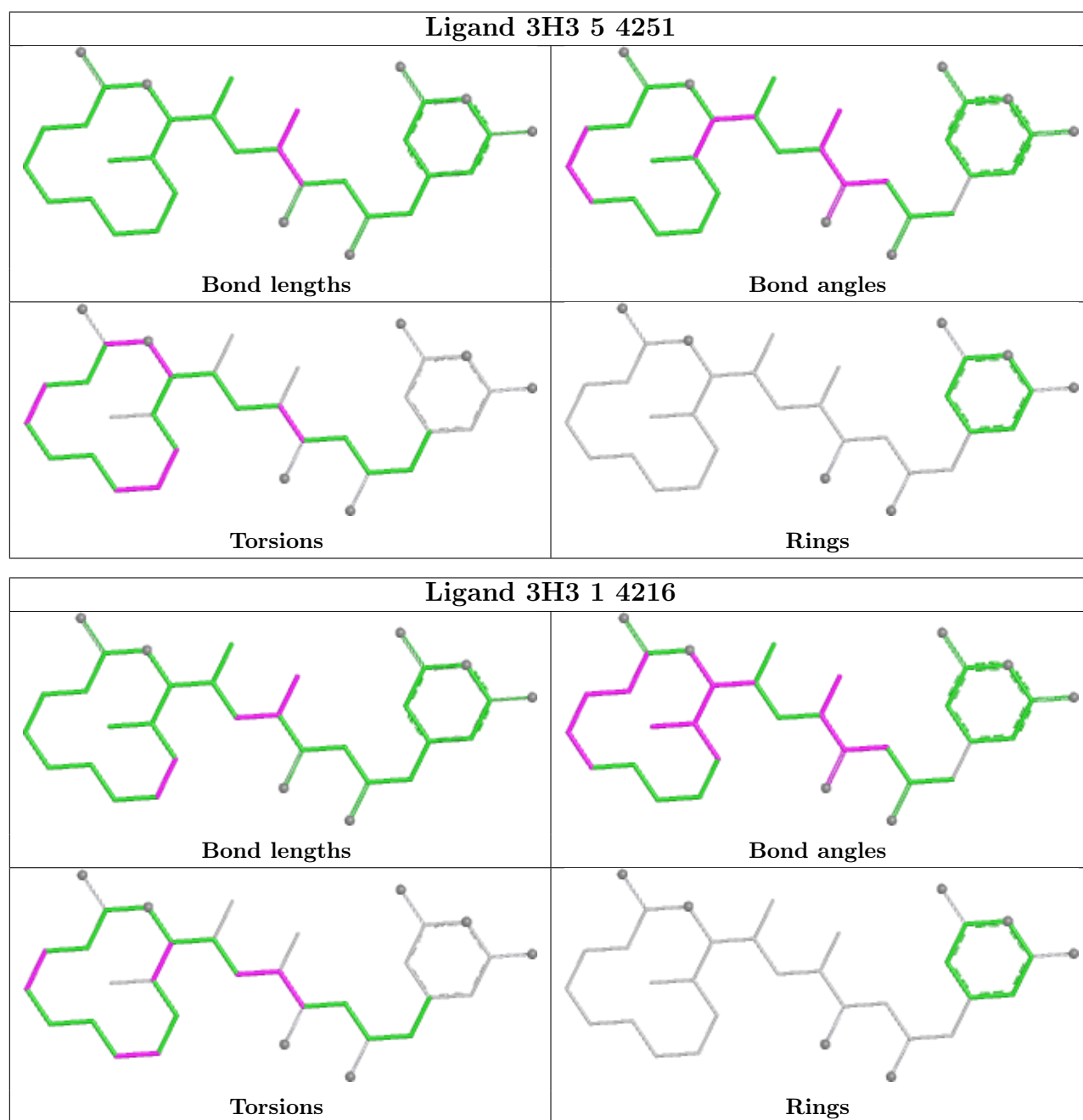
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | C3    | 202  | OHX  | 1       | 0            |
| 86  | 1     | 4103 | OHX  | 1       | 0            |
| 86  | 5     | 3906 | OHX  | 2       | 0            |
| 86  | 5     | 4125 | OHX  | 1       | 0            |
| 86  | 5     | 4214 | OHX  | 1       | 0            |
| 86  | 1     | 3924 | OHX  | 1       | 0            |
| 86  | Q2    | 503  | OHX  | 2       | 0            |
| 86  | 1     | 4198 | OHX  | 1       | 0            |
| 86  | 1     | 4184 | OHX  | 3       | 0            |
| 86  | c3    | 201  | OHX  | 3       | 0            |
| 86  | 5     | 3999 | OHX  | 1       | 0            |
| 86  | 6     | 2121 | OHX  | 8       | 0            |
| 86  | 1     | 4006 | OHX  | 1       | 0            |
| 86  | 1     | 4196 | OHX  | 1       | 0            |
| 86  | 2     | 2087 | OHX  | 1       | 0            |
| 86  | 7     | 218  | OHX  | 6       | 0            |
| 86  | M7    | 207  | OHX  | 1       | 0            |
| 86  | m0    | 302  | OHX  | 1       | 0            |
| 86  | 2     | 2079 | OHX  | 1       | 0            |
| 86  | 6     | 2182 | OHX  | 1       | 0            |
| 86  | 8     | 223  | OHX  | 6       | 0            |
| 86  | 1     | 4143 | OHX  | 6       | 0            |
| 86  | 1     | 3958 | OHX  | 1       | 0            |
| 86  | L4    | 404  | OHX  | 2       | 0            |
| 86  | 5     | 4055 | OHX  | 6       | 0            |
| 86  | C1    | 201  | OHX  | 7       | 0            |
| 86  | 6     | 2195 | OHX  | 1       | 0            |
| 86  | 6     | 2071 | OHX  | 1       | 0            |
| 86  | 6     | 2151 | OHX  | 1       | 0            |
| 86  | 5     | 4249 | OHX  | 1       | 0            |
| 86  | s1    | 302  | OHX  | 1       | 0            |
| 86  | 5     | 4081 | OHX  | 4       | 0            |
| 86  | 1     | 4178 | OHX  | 1       | 0            |
| 86  | L3    | 403  | OHX  | 1       | 0            |
| 86  | 5     | 4178 | OHX  | 2       | 0            |
| 86  | 1     | 4037 | OHX  | 1       | 0            |
| 86  | 1     | 4065 | OHX  | 8       | 0            |
| 86  | 2     | 2099 | OHX  | 7       | 0            |
| 86  | 5     | 4190 | OHX  | 6       | 0            |
| 86  | 1     | 4125 | OHX  | 1       | 0            |
| 86  | 6     | 2128 | OHX  | 2       | 0            |
| 86  | 2     | 2146 | OHX  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | 5     | 4152 | OHX  | 1       | 0            |
| 86  | 1     | 4144 | OHX  | 1       | 0            |
| 86  | 6     | 2156 | OHX  | 2       | 0            |
| 86  | 2     | 2048 | OHX  | 1       | 0            |
| 86  | 1     | 4172 | OHX  | 1       | 0            |
| 86  | 5     | 4230 | OHX  | 2       | 0            |
| 86  | M9    | 202  | OHX  | 1       | 0            |
| 86  | 1     | 3986 | OHX  | 2       | 0            |
| 86  | 5     | 4023 | OHX  | 3       | 0            |
| 86  | 1     | 4194 | OHX  | 1       | 0            |
| 86  | 2     | 2063 | OHX  | 1       | 0            |
| 86  | 5     | 4052 | OHX  | 1       | 0            |
| 86  | 5     | 4099 | OHX  | 1       | 0            |
| 86  | 1     | 4031 | OHX  | 2       | 0            |
| 86  | 5     | 4219 | OHX  | 1       | 0            |
| 86  | 1     | 3938 | OHX  | 1       | 0            |
| 86  | 5     | 4049 | OHX  | 1       | 0            |
| 86  | 1     | 3915 | OHX  | 1       | 0            |
| 86  | 2     | 2054 | OHX  | 1       | 0            |
| 86  | 6     | 2146 | OHX  | 1       | 0            |
| 86  | 5     | 4059 | OHX  | 1       | 0            |
| 86  | 1     | 3995 | OHX  | 1       | 0            |
| 86  | 5     | 4199 | OHX  | 3       | 0            |
| 86  | 2     | 2093 | OHX  | 2       | 0            |
| 86  | 5     | 4092 | OHX  | 1       | 0            |
| 86  | 2     | 2095 | OHX  | 1       | 0            |
| 86  | 1     | 3955 | OHX  | 3       | 0            |
| 86  | 4     | 223  | OHX  | 1       | 0            |
| 86  | 2     | 2046 | OHX  | 1       | 0            |
| 86  | 6     | 2122 | OHX  | 1       | 0            |
| 86  | c1    | 202  | OHX  | 7       | 0            |
| 86  | 5     | 4061 | OHX  | 1       | 0            |
| 86  | 1     | 4002 | OHX  | 2       | 0            |
| 86  | 1     | 3896 | OHX  | 1       | 0            |
| 86  | 1     | 4128 | OHX  | 1       | 0            |
| 86  | 1     | 4098 | OHX  | 1       | 0            |
| 86  | 1     | 4142 | OHX  | 3       | 0            |
| 86  | 1     | 3964 | OHX  | 7       | 0            |
| 86  | 1     | 4089 | OHX  | 4       | 0            |
| 86  | c5    | 201  | OHX  | 2       | 0            |
| 86  | 6     | 2125 | OHX  | 1       | 0            |
| 86  | 6     | 2165 | OHX  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34  | SR    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | SR    | 161:LYS   | C      | 162:ALA   | N      | 0.66         |
| 1     | SR    | 160:GLU   | C      | 161:LYS   | N      | 0.45         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | 2     | 1750/1800 (97%) | 0.30   | 97 (5%) 30 23 | 40, 69, 136, 230      | 0     |
| 1   | 6     | 1795/1800 (99%) | 0.17   | 94 (5%) 33 25 | 30, 58, 149, 237      | 0     |
| 2   | S0    | 206/251 (82%)   | 1.29   | 38 (18%) 3 2  | 73, 88, 101, 127      | 0     |
| 2   | s0    | 206/251 (82%)   | 0.74   | 20 (9%) 13 10 | 54, 71, 86, 92        | 0     |
| 3   | S1    | 214/254 (84%)   | 1.44   | 49 (22%) 2 1  | 79, 109, 140, 148     | 0     |
| 3   | s1    | 216/254 (85%)   | 0.49   | 7 (3%) 50 40  | 53, 65, 88, 96        | 0     |
| 4   | S2    | 217/253 (85%)   | 0.74   | 14 (6%) 25 18 | 54, 68, 83, 96        | 0     |
| 4   | s2    | 217/253 (85%)   | 0.29   | 7 (3%) 50 40  | 42, 56, 69, 78        | 0     |
| 5   | S3    | 223/239 (93%)   | 0.82   | 21 (9%) 14 10 | 59, 72, 92, 108       | 0     |
| 5   | s3    | 223/239 (93%)   | 0.63   | 12 (5%) 31 24 | 55, 76, 98, 104       | 0     |
| 6   | S4    | 260/260 (100%)  | 0.60   | 9 (3%) 47 38  | 47, 69, 80, 108       | 0     |
| 6   | s4    | 260/260 (100%)  | 0.21   | 5 (1%) 66 57  | 37, 58, 69, 100       | 0     |
| 7   | S5    | 206/224 (91%)   | 1.09   | 23 (11%) 10 7 | 73, 92, 107, 120      | 0     |
| 7   | s5    | 206/224 (91%)   | 1.00   | 23 (11%) 10 7 | 56, 77, 101, 113      | 0     |
| 8   | S6    | 226/236 (95%)   | 1.17   | 39 (17%) 4 3  | 49, 82, 98, 126       | 0     |
| 8   | s6    | 218/236 (92%)   | 0.77   | 19 (8%) 16 11 | 38, 66, 87, 107       | 0     |
| 9   | S7    | 184/189 (97%)   | 1.26   | 27 (14%) 6 4  | 65, 92, 123, 131      | 0     |
| 9   | s7    | 186/189 (98%)   | 1.18   | 28 (15%) 5 4  | 49, 78, 112, 122      | 0     |
| 10  | S8    | 188/200 (94%)   | 0.66   | 15 (7%) 18 13 | 40, 55, 89, 104       | 0     |
| 10  | s8    | 188/200 (94%)   | 0.62   | 12 (6%) 25 18 | 33, 52, 95, 111       | 0     |
| 11  | S9    | 185/196 (94%)   | 0.90   | 16 (8%) 16 12 | 64, 77, 113, 146      | 0     |
| 11  | s9    | 185/196 (94%)   | 0.24   | 3 (1%) 70 61  | 49, 62, 99, 125       | 0     |
| 12  | C0    | 96/105 (91%)    | 0.81   | 10 (10%) 11 8 | 63, 83, 110, 128      | 0     |
| 12  | c0    | 96/105 (91%)    | 1.09   | 18 (18%) 3 2  | 69, 99, 122, 140      | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|---------|-----------------------|-------|
| 13  | C1    | 155/155 (100%) | 0.78   | 17 (10%) | 10 8    | 43, 53, 103, 117      | 0     |
| 13  | c1    | 146/155 (94%)  | 0.72   | 13 (8%)  | 15 11   | 34, 48, 76, 96        | 0     |
| 14  | C2    | 124/142 (87%)  | 1.18   | 22 (17%) | 4 3     | 105, 118, 138, 151    | 0     |
| 14  | c2    | 124/142 (87%)  | 1.60   | 29 (23%) | 2 1     | 139, 159, 175, 184    | 0     |
| 15  | C3    | 150/150 (100%) | 0.62   | 5 (3%)   | 49 39   | 50, 67, 80, 86        | 0     |
| 15  | c3    | 150/150 (100%) | 0.50   | 7 (4%)   | 36 29   | 40, 55, 71, 85        | 0     |
| 16  | C4    | 127/136 (93%)  | 1.46   | 30 (23%) | 2 1     | 54, 113, 128, 131     | 0     |
| 16  | c4    | 128/136 (94%)  | 0.78   | 10 (7%)  | 19 14   | 38, 71, 80, 83        | 0     |
| 17  | C5    | 124/141 (87%)  | 0.74   | 13 (10%) | 11 8    | 58, 72, 108, 128      | 0     |
| 17  | c5    | 135/141 (95%)  | 0.93   | 15 (11%) | 10 7    | 58, 74, 98, 120       | 0     |
| 18  | C6    | 141/142 (99%)  | 0.82   | 14 (9%)  | 13 9    | 62, 82, 87, 89        | 0     |
| 18  | c6    | 142/142 (100%) | 0.94   | 20 (14%) | 6 5     | 50, 71, 84, 105       | 0     |
| 19  | C7    | 120/136 (88%)  | 1.36   | 30 (25%) | 2 1     | 68, 85, 111, 113      | 0     |
| 19  | c7    | 117/136 (86%)  | 0.97   | 19 (16%) | 4 4     | 59, 72, 98, 109       | 0     |
| 20  | C8    | 145/145 (100%) | 0.78   | 12 (8%)  | 17 12   | 58, 80, 105, 114      | 0     |
| 20  | c8    | 145/145 (100%) | 0.52   | 9 (6%)   | 26 20   | 55, 65, 90, 103       | 0     |
| 21  | C9    | 143/143 (100%) | 0.68   | 6 (4%)   | 40 32   | 66, 80, 94, 105       | 0     |
| 21  | c9    | 143/143 (100%) | 0.54   | 4 (2%)   | 55 45   | 51, 64, 82, 98        | 0     |
| 22  | D0    | 107/120 (89%)  | 1.23   | 25 (23%) | 2 1     | 56, 87, 118, 128      | 0     |
| 22  | d0    | 110/120 (91%)  | 1.25   | 24 (21%) | 2 2     | 50, 82, 120, 132      | 0     |
| 23  | D1    | 87/87 (100%)   | 0.95   | 9 (10%)  | 12 9    | 69, 75, 92, 99        | 0     |
| 23  | d1    | 87/87 (100%)   | 0.20   | 0        | 100 100 | 53, 59, 77, 88        | 0     |
| 24  | D2    | 129/129 (100%) | 0.57   | 2 (1%)   | 70 61   | 52, 62, 68, 78        | 0     |
| 24  | d2    | 129/129 (100%) | 0.10   | 0        | 100 100 | 37, 47, 53, 61        | 0     |
| 25  | D3    | 144/144 (100%) | 0.28   | 4 (2%)   | 55 45   | 43, 49, 59, 73        | 0     |
| 25  | d3    | 144/144 (100%) | -0.13  | 1 (0%)   | 84 77   | 33, 38, 52, 65        | 0     |
| 26  | D4    | 134/134 (100%) | 0.74   | 14 (10%) | 11 8    | 59, 82, 97, 105       | 0     |
| 26  | d4    | 134/134 (100%) | 0.52   | 9 (6%)   | 24 17   | 46, 66, 81, 100       | 0     |
| 27  | D5    | 70/107 (65%)   | 1.39   | 19 (27%) | 1 1     | 87, 103, 115, 121     | 0     |
| 27  | d5    | 69/107 (64%)   | 1.16   | 12 (17%) | 4 3     | 66, 87, 99, 101       | 0     |
| 28  | D6    | 97/97 (100%)   | 1.07   | 15 (15%) | 5 4     | 59, 74, 129, 133      | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | d6    | 97/97 (100%)    | 0.64   | 7 (7%) 21 16   | 43, 55, 84, 93        | 0     |
| 29  | D7    | 81/81 (100%)    | 0.88   | 6 (7%) 20 15   | 64, 79, 113, 123      | 0     |
| 29  | d7    | 81/81 (100%)    | 0.94   | 11 (13%) 7 5   | 49, 66, 106, 109      | 0     |
| 30  | D8    | 63/66 (95%)     | 1.42   | 11 (17%) 4 3   | 89, 104, 118, 130     | 0     |
| 30  | d8    | 63/66 (95%)     | 1.41   | 12 (19%) 3 2   | 74, 89, 103, 112      | 0     |
| 31  | D9    | 53/55 (96%)     | 0.37   | 4 (7%) 20 15   | 56, 60, 80, 89        | 0     |
| 31  | d9    | 53/55 (96%)     | 0.52   | 4 (7%) 20 15   | 52, 58, 95, 109       | 0     |
| 32  | E0    | 60/60 (100%)    | 0.70   | 8 (13%) 7 5    | 47, 79, 115, 121      | 0     |
| 33  | E1    | 71/76 (93%)     | 1.37   | 17 (23%) 2 1   | 91, 102, 113, 115     | 0     |
| 33  | e1    | 76/76 (100%)    | 1.67   | 22 (28%) 1 1   | 117, 130, 148, 153    | 0     |
| 34  | SR    | 318/318 (100%)  | 0.71   | 21 (6%) 24 18  | 55, 87, 106, 129      | 0     |
| 34  | sR    | 318/318 (100%)  | 0.93   | 29 (9%) 15 11  | 73, 91, 107, 124      | 0     |
| 35  | SM    | 159/273 (58%)   | 1.29   | 38 (23%) 2 1   | 51, 73, 118, 120      | 0     |
| 35  | sM    | 104/273 (38%)   | 1.16   | 25 (24%) 2 1   | 40, 75, 155, 158      | 0     |
| 36  | 1     | 3149/3396 (92%) | -0.19  | 113 (3%) 46 37 | 17, 37, 108, 219      | 0     |
| 36  | 5     | 3150/3396 (92%) | -0.23  | 100 (3%) 50 40 | 17, 36, 101, 220      | 0     |
| 37  | 3     | 121/121 (100%)  | -0.40  | 82 75          | 28, 53, 70, 75        | 0     |
| 37  | 7     | 121/121 (100%)  | -0.48  | 69 60          | 24, 40, 51, 59        | 0     |
| 38  | 4     | 158/158 (100%)  | -0.50  | 58 48          | 22, 40, 74, 105       | 0     |
| 38  | 8     | 158/158 (100%)  | -0.30  | 50 40          | 27, 46, 80, 102       | 0     |
| 39  | L2    | 252/253 (99%)   | -0.11  | 82 75          | 20, 35, 50, 58        | 0     |
| 39  | l2    | 252/253 (99%)   | 0.03   | 50 40          | 21, 37, 55, 62        | 0     |
| 40  | L3    | 386/386 (100%)  | -0.13  | 67 58          | 23, 41, 54, 87        | 0     |
| 40  | l3    | 386/386 (100%)  | -0.32  | 82 75          | 17, 30, 42, 73        | 0     |
| 41  | L4    | 361/361 (100%)  | -0.03  | 55 45          | 19, 33, 49, 57        | 0     |
| 41  | l4    | 361/361 (100%)  | 0.23   | 39 31          | 21, 38, 55, 62        | 0     |
| 42  | L5    | 296/296 (100%)  | 0.25   | 48 39          | 37, 59, 77, 103       | 0     |
| 42  | l5    | 294/296 (99%)   | 0.01   | 51 41          | 29, 43, 66, 101       | 0     |
| 43  | L6    | 156/175 (89%)   | 0.00   | 66 57          | 28, 35, 53, 69        | 0     |
| 43  | l6    | 157/175 (89%)   | 0.18   | 44 35          | 30, 38, 56, 68        | 0     |
| 44  | L7    | 222/243 (91%)   | -0.12  | 67 58          | 21, 29, 54, 92        | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44  | l7    | 223/243 (91%)  | -0.14  | 5 (2%) 62 52  | 20, 28, 65, 105       | 0     |
| 45  | L8    | 233/255 (91%)  | 0.40   | 15 (6%) 25 18 | 42, 54, 88, 105       | 0     |
| 45  | l8    | 231/255 (90%)  | 0.65   | 15 (6%) 25 18 | 51, 63, 88, 93        | 0     |
| 46  | L9    | 191/191 (100%) | 0.10   | 1 (0%) 87 82  | 37, 48, 60, 76        | 0     |
| 46  | l9    | 191/191 (100%) | -0.01  | 5 (2%) 57 47  | 27, 35, 54, 75        | 0     |
| 47  | M0    | 211/220 (95%)  | 0.02   | 6 (2%) 55 45  | 24, 38, 72, 91        | 0     |
| 47  | m0    | 213/220 (96%)  | 0.21   | 12 (5%) 30 23 | 25, 41, 64, 83        | 0     |
| 48  | M1    | 169/173 (97%)  | 0.40   | 4 (2%) 59 49  | 45, 63, 76, 84        | 0     |
| 48  | m1    | 169/173 (97%)  | 0.12   | 4 (2%) 59 49  | 32, 48, 60, 71        | 0     |
| 49  | M3    | 193/198 (97%)  | -0.01  | 4 (2%) 63 54  | 21, 39, 73, 98        | 0     |
| 49  | m3    | 194/198 (97%)  | 0.26   | 8 (4%) 41 33  | 27, 47, 80, 102       | 0     |
| 50  | M4    | 136/137 (99%)  | 0.11   | 4 (2%) 53 43  | 31, 38, 51, 59        | 0     |
| 50  | m4    | 137/137 (100%) | 0.08   | 6 (4%) 39 31  | 28, 33, 51, 62        | 0     |
| 51  | M5    | 203/203 (100%) | -0.27  | 0 100 100     | 20, 34, 42, 49        | 0     |
| 51  | m5    | 203/203 (100%) | -0.16  | 0 100 100     | 25, 41, 51, 56        | 0     |
| 52  | M6    | 197/198 (99%)  | -0.08  | 5 (2%) 58 48  | 22, 29, 48, 54        | 0     |
| 52  | m6    | 197/198 (99%)  | -0.18  | 5 (2%) 58 48  | 18, 23, 47, 53        | 0     |
| 53  | M7    | 183/183 (100%) | 0.29   | 16 (8%) 16 11 | 25, 32, 82, 114       | 0     |
| 53  | m7    | 155/183 (84%)  | -0.25  | 2 (1%) 75 66  | 21, 28, 40, 64        | 0     |
| 54  | M8    | 185/185 (100%) | -0.18  | 0 100 100     | 22, 31, 44, 56        | 0     |
| 54  | m8    | 185/185 (100%) | -0.10  | 1 (0%) 87 82  | 26, 37, 46, 52        | 0     |
| 55  | M9    | 188/188 (100%) | 0.58   | 18 (9%) 13 10 | 38, 51, 127, 140      | 0     |
| 55  | m9    | 188/188 (100%) | 0.41   | 11 (5%) 28 21 | 34, 45, 105, 122      | 0     |
| 56  | N0    | 172/172 (100%) | 0.01   | 3 (1%) 69 60  | 29, 36, 48, 54        | 0     |
| 56  | n0    | 172/172 (100%) | -0.01  | 5 (2%) 53 43  | 23, 30, 40, 48        | 0     |
| 57  | N1    | 159/159 (100%) | 0.03   | 3 (1%) 66 57  | 25, 35, 71, 78        | 0     |
| 57  | n1    | 159/159 (100%) | -0.12  | 1 (0%) 85 80  | 25, 31, 64, 70        | 0     |
| 58  | N2    | 100/120 (83%)  | 0.96   | 10 (10%) 12 9 | 67, 81, 92, 101       | 0     |
| 58  | n2    | 98/120 (81%)   | 0.76   | 7 (7%) 22 16  | 58, 70, 80, 81        | 0     |
| 59  | N3    | 136/136 (100%) | -0.04  | 5 (3%) 45 36  | 27, 37, 50, 57        | 0     |
| 59  | n3    | 136/136 (100%) | -0.17  | 3 (2%) 62 52  | 19, 28, 42, 45        | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 60  | N4    | 98/155 (63%)   | 1.71   | 36 (36%) 1 0  | 37, 48, 127, 130      | 0     |
| 60  | n4    | 135/155 (87%)  | 1.25   | 37 (27%) 1 1  | 28, 74, 108, 124      | 0     |
| 61  | N5    | 121/141 (85%)  | -0.04  | 1 (0%) 82 75  | 34, 46, 61, 83        | 0     |
| 61  | n5    | 120/141 (85%)  | 0.20   | 1 (0%) 82 75  | 36, 49, 67, 72        | 0     |
| 62  | N6    | 126/126 (100%) | -0.28  | 1 (0%) 82 75  | 27, 42, 53, 61        | 0     |
| 62  | n6    | 126/126 (100%) | -0.05  | 1 (0%) 82 75  | 32, 45, 60, 65        | 0     |
| 63  | N7    | 135/135 (100%) | 0.35   | 2 (1%) 72 63  | 53, 66, 80, 88        | 0     |
| 63  | n7    | 135/135 (100%) | 0.68   | 5 (3%) 45 36  | 57, 72, 91, 99        | 0     |
| 64  | N8    | 148/148 (100%) | -0.12  | 2 (1%) 73 64  | 18, 32, 54, 63        | 0     |
| 64  | n8    | 148/148 (100%) | -0.02  | 0 100 100     | 19, 39, 56, 58        | 0     |
| 65  | N9    | 58/58 (100%)   | 0.45   | 5 (8%) 16 12  | 19, 39, 79, 90        | 0     |
| 65  | n9    | 58/58 (100%)   | 0.39   | 4 (6%) 23 16  | 19, 40, 59, 70        | 0     |
| 66  | O0    | 97/104 (93%)   | 0.25   | 5 (5%) 33 25  | 51, 60, 81, 85        | 0     |
| 66  | o0    | 100/104 (96%)  | 0.58   | 10 (10%) 12 9 | 54, 63, 88, 100       | 0     |
| 67  | O1    | 109/112 (97%)  | 0.22   | 7 (6%) 25 18  | 35, 48, 77, 91        | 0     |
| 67  | o1    | 109/112 (97%)  | 0.06   | 6 (5%) 30 23  | 28, 39, 72, 90        | 0     |
| 68  | O2    | 127/129 (98%)  | -0.12  | 3 (2%) 59 49  | 18, 30, 40, 56        | 0     |
| 68  | o2    | 127/129 (98%)  | -0.09  | 3 (2%) 59 49  | 19, 34, 46, 65        | 0     |
| 69  | O3    | 106/106 (100%) | -0.21  | 1 (0%) 81 74  | 23, 28, 47, 56        | 0     |
| 69  | o3    | 106/106 (100%) | -0.13  | 4 (3%) 44 35  | 20, 27, 51, 60        | 0     |
| 70  | O4    | 112/119 (94%)  | 0.36   | 5 (4%) 38 30  | 34, 49, 87, 100       | 0     |
| 70  | o4    | 112/119 (94%)  | 0.40   | 4 (3%) 46 37  | 34, 49, 85, 93        | 0     |
| 71  | O5    | 119/119 (100%) | 0.11   | 4 (3%) 48 39  | 32, 49, 55, 58        | 0     |
| 71  | o5    | 119/119 (100%) | 0.19   | 2 (1%) 69 60  | 40, 54, 62, 68        | 0     |
| 72  | O6    | 99/99 (100%)   | 0.25   | 4 (4%) 42 33  | 36, 45, 72, 86        | 0     |
| 72  | o6    | 99/99 (100%)   | 0.30   | 3 (3%) 52 42  | 45, 55, 74, 90        | 0     |
| 73  | O7    | 87/87 (100%)   | -0.11  | 2 (2%) 61 51  | 23, 28, 50, 71        | 0     |
| 73  | o7    | 87/87 (100%)   | -0.14  | 1 (1%) 78 70  | 24, 30, 60, 95        | 0     |
| 74  | O8    | 77/77 (100%)   | 0.48   | 2 (2%) 57 47  | 57, 69, 90, 98        | 0     |
| 74  | o8    | 77/77 (100%)   | 0.51   | 3 (3%) 43 34  | 57, 69, 87, 91        | 0     |
| 75  | O9    | 50/50 (100%)   | 0.06   | 2 (4%) 42 33  | 32, 35, 44, 49        | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 75  | o9    | 50/50 (100%)      | 0.01   | 0 100 100       | 35, 38, 48, 52        | 0     |
| 76  | Q0    | 52/52 (100%)      | -0.15  | 1 (1%) 66 57    | 33, 38, 53, 64        | 0     |
| 76  | q0    | 52/52 (100%)      | -0.29  | 1 (1%) 66 57    | 23, 26, 38, 44        | 0     |
| 77  | Q1    | 25/25 (100%)      | 0.16   | 0 100 100       | 41, 43, 47, 52        | 0     |
| 77  | q1    | 25/25 (100%)      | 0.03   | 0 100 100       | 31, 35, 44, 50        | 0     |
| 78  | Q2    | 105/105 (100%)    | 0.05   | 5 (4%) 35 28    | 22, 38, 56, 82        | 0     |
| 78  | q2    | 105/105 (100%)    | -0.08  | 1 (0%) 79 72    | 26, 38, 51, 78        | 0     |
| 79  | Q3    | 91/91 (100%)      | 0.03   | 2 (2%) 62 52    | 28, 38, 53, 66        | 0     |
| 79  | q3    | 91/91 (100%)      | 0.08   | 2 (2%) 62 52    | 26, 38, 51, 59        | 0     |
| 80  | e0    | 62/62 (100%)      | 0.43   | 3 (4%) 35 28    | 46, 64, 97, 99        | 0     |
| 81  | m2    | 0/160             | -      | -               | -                     | -     |
| 82  | p0    | 143/311 (45%)     | 1.75   | 51 (35%) 1 0    | 72, 90, 159, 170      | 0     |
| 83  | p1    | 0/47              | -      | -               | -                     | -     |
| 84  | p2    | 0/46              | -      | -               | -                     | -     |
| All | All   | 33063/35344 (93%) | 0.27   | 1949 (5%) 28 21 | 17, 52, 109, 237      | 0     |

All (1949) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 5     | 2871 | G    | 12.1 |
| 36  | 5     | 2873 | U    | 11.2 |
| 13  | c1    | 3    | THR  | 11.1 |
| 60  | N4    | 86   | SER  | 10.7 |
| 36  | 5     | 2403 | G    | 9.8  |
| 36  | 1     | 2402 | A    | 9.7  |
| 36  | 5     | 2874 | G    | 9.4  |
| 60  | N4    | 88   | ASP  | 9.3  |
| 60  | N4    | 76   | VAL  | 9.2  |
| 36  | 1     | 2871 | G    | 9.0  |
| 36  | 5     | 2402 | A    | 8.8  |
| 36  | 1     | 2401 | A    | 8.6  |
| 60  | n4    | 68   | ALA  | 8.4  |
| 60  | N4    | 89   | LEU  | 8.2  |
| 47  | m0    | 111  | LEU  | 8.1  |
| 36  | 1     | 2403 | G    | 8.0  |
| 7   | S5    | 152  | GLY  | 8.0  |
| 36  | 1     | 2873 | U    | 7.9  |
| 36  | 1     | 2874 | G    | 7.7  |

Continued on next page...

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | 1            | 2404       | A           | 7.6         |
| 82         | p0           | 192        | ASP         | 7.6         |
| 60         | N4           | 75         | THR         | 7.4         |
| 7          | S5           | 37         | GLN         | 7.3         |
| 60         | N4           | 69         | LYS         | 7.3         |
| 7          | S5           | 36         | ALA         | 7.3         |
| 36         | 5            | 2401       | A           | 7.2         |
| 13         | C1           | 145        | ALA         | 7.2         |
| 13         | C1           | 146        | ALA         | 7.2         |
| 17         | c5           | 4          | ALA         | 7.1         |
| 7          | s5           | 37         | GLN         | 7.1         |
| 13         | c1           | 5          | LEU         | 7.1         |
| 13         | C1           | 152        | GLN         | 7.0         |
| 1          | 6            | 663        | U           | 6.8         |
| 60         | N4           | 72         | SER         | 6.7         |
| 1          | 6            | 662        | U           | 6.7         |
| 56         | n0           | 1          | MET         | 6.4         |
| 35         | SM           | 9          | GLY         | 6.4         |
| 56         | N0           | 1          | MET         | 6.4         |
| 53         | M7           | 184        | ALA         | 6.3         |
| 41         | l4           | 67         | THR         | 6.2         |
| 47         | m0           | 221        | ALA         | 6.1         |
| 53         | M7           | 161        | ALA         | 6.1         |
| 49         | m3           | 195        | ALA         | 6.1         |
| 13         | C1           | 2          | SER         | 6.1         |
| 60         | n4           | 67         | VAL         | 6.0         |
| 60         | n4           | 69         | LYS         | 6.0         |
| 1          | 6            | 1491       | U           | 6.0         |
| 36         | 5            | 2404       | A           | 6.0         |
| 23         | D1           | 10         | GLU         | 5.9         |
| 53         | M7           | 165        | VAL         | 5.9         |
| 22         | d0           | 97         | VAL         | 5.8         |
| 1          | 2            | 238        | U           | 5.8         |
| 35         | SM           | 87         | THR         | 5.8         |
| 17         | c5           | 5          | VAL         | 5.7         |
| 36         | 1            | 1349       | G           | 5.7         |
| 35         | SM           | 11         | ASP         | 5.7         |
| 36         | 1            | 2872       | A           | 5.7         |
| 47         | m0           | 103        | LEU         | 5.7         |
| 75         | O9           | 2          | ALA         | 5.7         |
| 19         | C7           | 123        | ASN         | 5.7         |
| 33         | e1           | 80         | ARG         | 5.6         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | C1    | 3    | THR  | 5.6  |
| 13  | C1    | 148  | LYS  | 5.6  |
| 36  | 1     | 1952 | G    | 5.6  |
| 60  | n4    | 70   | LYS  | 5.5  |
| 17  | c5    | 133  | ALA  | 5.5  |
| 13  | C1    | 147  | ALA  | 5.5  |
| 60  | N4    | 77   | LYS  | 5.5  |
| 16  | C4    | 15   | GLY  | 5.5  |
| 55  | M9    | 189  | ALA  | 5.5  |
| 4   | s2    | 90   | THR  | 5.4  |
| 35  | SM    | 88   | ARG  | 5.4  |
| 9   | s7    | 12   | ALA  | 5.4  |
| 79  | q3    | 2    | ALA  | 5.4  |
| 3   | S1    | 25   | THR  | 5.4  |
| 1   | 2     | 320  | U    | 5.3  |
| 60  | n4    | 65   | GLU  | 5.3  |
| 1   | 6     | 794  | U    | 5.2  |
| 19  | c7    | 96   | SER  | 5.2  |
| 36  | 5     | 2872 | A    | 5.2  |
| 12  | C0    | 96   | ASN  | 5.2  |
| 7   | s5    | 151  | GLY  | 5.2  |
| 17  | c5    | 134  | THR  | 5.2  |
| 1   | 6     | 1800 | A    | 5.2  |
| 12  | C0    | 89   | ALA  | 5.2  |
| 13  | c1    | 144  | ALA  | 5.2  |
| 2   | S0    | 207  | PRO  | 5.2  |
| 36  | 1     | 1571 | A    | 5.1  |
| 41  | L4    | 69   | ARG  | 5.1  |
| 56  | n0    | 17   | GLU  | 5.1  |
| 60  | N4    | 73   | ARG  | 5.1  |
| 9   | s7    | 3    | ALA  | 5.1  |
| 60  | N4    | 95   | SER  | 5.1  |
| 1   | 6     | 678  | A    | 5.1  |
| 2   | S0    | 190  | ASP  | 5.0  |
| 13  | c1    | 145  | ALA  | 5.0  |
| 1   | 2     | 913  | G    | 5.0  |
| 36  | 1     | 1581 | C    | 5.0  |
| 35  | SM    | 85   | SER  | 5.0  |
| 36  | 1     | 2205 | U    | 5.0  |
| 13  | c1    | 4    | GLU  | 5.0  |
| 60  | N4    | 92   | GLU  | 5.0  |
| 36  | 1     | 2522 | G    | 5.0  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 68         | O2           | 128        | LEU         | 4.9         |
| 45         | L8           | 256        | ALA         | 4.9         |
| 60         | n4           | 109        | LEU         | 4.9         |
| 71         | o5           | 120        | ALA         | 4.9         |
| 73         | O7           | 88         | ALA         | 4.9         |
| 36         | 1            | 1569       | U           | 4.9         |
| 1          | 2            | 506        | A           | 4.9         |
| 19         | c7           | 97         | ASN         | 4.9         |
| 60         | N4           | 68         | ALA         | 4.8         |
| 59         | n3           | 2          | SER         | 4.8         |
| 50         | m4           | 8          | LYS         | 4.8         |
| 36         | 1            | 1352       | A           | 4.8         |
| 36         | 1            | 2207       | A           | 4.8         |
| 82         | p0           | 107        | ALA         | 4.8         |
| 20         | c8           | 3          | LEU         | 4.8         |
| 36         | 5            | 1349       | G           | 4.8         |
| 73         | o7           | 88         | ALA         | 4.8         |
| 1          | 6            | 664        | U           | 4.8         |
| 22         | D0           | 19         | ILE         | 4.7         |
| 16         | c4           | 125        | SER         | 4.7         |
| 14         | c2           | 123        | VAL         | 4.7         |
| 52         | m6           | 184        | THR         | 4.7         |
| 37         | 7            | 73         | C           | 4.7         |
| 7          | s5           | 153        | GLY         | 4.7         |
| 41         | l4           | 65         | TRP         | 4.7         |
| 3          | S1           | 20         | VAL         | 4.7         |
| 45         | l8           | 124        | ASP         | 4.7         |
| 40         | L3           | 387        | LEU         | 4.7         |
| 7          | s5           | 155        | ALA         | 4.7         |
| 12         | c0           | 84         | GLU         | 4.7         |
| 36         | 5            | 1352       | A           | 4.7         |
| 38         | 8            | 81         | U           | 4.6         |
| 13         | C1           | 156        | PHE         | 4.6         |
| 13         | c1           | 146        | ALA         | 4.6         |
| 19         | C7           | 97         | ASN         | 4.6         |
| 19         | c7           | 95         | ARG         | 4.6         |
| 33         | E1           | 87         | THR         | 4.6         |
| 29         | D7           | 38         | PRO         | 4.6         |
| 33         | e1           | 147        | VAL         | 4.6         |
| 53         | M7           | 166        | VAL         | 4.6         |
| 9          | S7           | 34         | LEU         | 4.6         |
| 19         | C7           | 126        | ALA         | 4.6         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | e1    | 152  | ALA  | 4.6  |
| 60  | N4    | 79   | GLN  | 4.6  |
| 36  | 5     | 2971 | A    | 4.5  |
| 33  | e1    | 77   | GLY  | 4.5  |
| 68  | o2    | 128  | LEU  | 4.5  |
| 28  | D6    | 98   | PRO  | 4.5  |
| 56  | n0    | 2    | ALA  | 4.5  |
| 55  | m9    | 189  | ALA  | 4.5  |
| 35  | SM    | 175  | ASP  | 4.5  |
| 36  | 1     | 1955 | U    | 4.5  |
| 36  | 1     | 1350 | A    | 4.5  |
| 18  | C6    | 3    | ALA  | 4.5  |
| 55  | M9    | 131  | ALA  | 4.5  |
| 35  | SM    | 134  | ASP  | 4.5  |
| 41  | l4    | 61   | SER  | 4.5  |
| 82  | p0    | 218  | SER  | 4.5  |
| 11  | S9    | 95   | TYR  | 4.4  |
| 57  | N1    | 121  | ALA  | 4.4  |
| 41  | l4    | 62   | ALA  | 4.4  |
| 10  | s8    | 135  | LYS  | 4.4  |
| 10  | s8    | 200  | LYS  | 4.4  |
| 2   | s0    | 207  | PRO  | 4.4  |
| 9   | s7    | 4    | PRO  | 4.4  |
| 22  | d0    | 98   | GLN  | 4.4  |
| 34  | sR    | 107  | LYS  | 4.4  |
| 80  | e0    | 62   | VAL  | 4.4  |
| 55  | M9    | 185  | LEU  | 4.4  |
| 65  | n9    | 22   | LYS  | 4.4  |
| 9   | s7    | 187  | SER  | 4.3  |
| 60  | n4    | 72   | SER  | 4.3  |
| 1   | 2     | 794  | U    | 4.3  |
| 27  | d5    | 86   | GLU  | 4.3  |
| 35  | SM    | 84   | LYS  | 4.3  |
| 53  | M7    | 164  | LYS  | 4.3  |
| 17  | C5    | 11   | VAL  | 4.3  |
| 13  | c1    | 2    | SER  | 4.3  |
| 2   | S0    | 32   | HIS  | 4.3  |
| 30  | D8    | 44   | VAL  | 4.3  |
| 7   | s5    | 152  | GLY  | 4.3  |
| 36  | 1     | 2206 | G    | 4.3  |
| 22  | d0    | 120  | SER  | 4.3  |
| 60  | N4    | 93   | ARG  | 4.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | S8    | 152  | ILE  | 4.2  |
| 34  | SR    | 2    | ALA  | 4.2  |
| 82  | p0    | 105  | VAL  | 4.2  |
| 42  | L5    | 293  | LEU  | 4.2  |
| 22  | d0    | 18   | GLN  | 4.2  |
| 36  | 1     | 1568 | U    | 4.2  |
| 60  | N4    | 65   | GLU  | 4.2  |
| 5   | s3    | 217  | ILE  | 4.2  |
| 60  | N4    | 63   | ILE  | 4.2  |
| 12  | c0    | 81   | ASN  | 4.2  |
| 42  | l5    | 270  | LYS  | 4.2  |
| 48  | m1    | 174  | LYS  | 4.2  |
| 60  | N4    | 96   | LEU  | 4.2  |
| 1   | 6     | 676  | G    | 4.2  |
| 47  | M0    | 220  | GLN  | 4.2  |
| 17  | c5    | 7    | ALA  | 4.2  |
| 10  | S8    | 21   | PHE  | 4.2  |
| 14  | c2    | 126  | TRP  | 4.1  |
| 2   | S0    | 29   | VAL  | 4.1  |
| 12  | c0    | 98   | THR  | 4.1  |
| 41  | l4    | 69   | ARG  | 4.1  |
| 6   | S4    | 261  | LEU  | 4.1  |
| 82  | p0    | 210  | VAL  | 4.1  |
| 26  | D4    | 134  | ALA  | 4.1  |
| 36  | 1     | 1351 | U    | 4.1  |
| 32  | E0    | 53   | LYS  | 4.1  |
| 36  | 5     | 1350 | A    | 4.1  |
| 35  | SM    | 89   | ARG  | 4.1  |
| 9   | S7    | 38   | LEU  | 4.1  |
| 20  | C8    | 17   | LEU  | 4.1  |
| 46  | l9    | 191  | LEU  | 4.1  |
| 33  | e1    | 150  | VAL  | 4.1  |
| 35  | sM    | 167  | PRO  | 4.1  |
| 26  | d4    | 134  | ALA  | 4.1  |
| 9   | s7    | 2    | SER  | 4.1  |
| 27  | D5    | 88   | ILE  | 4.1  |
| 36  | 1     | 1570 | U    | 4.1  |
| 44  | L7    | 26   | VAL  | 4.1  |
| 60  | N4    | 81   | PRO  | 4.1  |
| 16  | c4    | 45   | GLY  | 4.1  |
| 12  | c0    | 94   | GLU  | 4.1  |
| 82  | p0    | 200  | SER  | 4.1  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | c7    | 121  | VAL  | 4.0  |
| 36  | 1     | 440  | A    | 4.0  |
| 5   | S3    | 3    | ALA  | 4.0  |
| 18  | C6    | 143  | ARG  | 4.0  |
| 22  | D0    | 120  | SER  | 4.0  |
| 82  | p0    | 217  | VAL  | 4.0  |
| 8   | S6    | 219  | ARG  | 4.0  |
| 19  | C7    | 95   | ARG  | 4.0  |
| 55  | m9    | 151  | ARG  | 4.0  |
| 60  | n4    | 66   | GLU  | 4.0  |
| 22  | D0    | 97   | VAL  | 4.0  |
| 33  | e1    | 78   | LYS  | 4.0  |
| 50  | m4    | 9    | ALA  | 4.0  |
| 8   | s6    | 169  | TYR  | 4.0  |
| 3   | S1    | 100  | PHE  | 4.0  |
| 29  | d7    | 41   | LEU  | 4.0  |
| 3   | S1    | 84   | ILE  | 4.0  |
| 36  | 5     | 1582 | C    | 4.0  |
| 45  | L8    | 116  | VAL  | 4.0  |
| 60  | N4    | 98   | PRO  | 4.0  |
| 82  | p0    | 184  | GLY  | 3.9  |
| 1   | 6     | 321  | C    | 3.9  |
| 82  | p0    | 197  | PHE  | 3.9  |
| 8   | S6    | 149  | LYS  | 3.9  |
| 68  | o2    | 16   | LYS  | 3.9  |
| 82  | p0    | 211  | SER  | 3.9  |
| 13  | C1    | 4    | GLU  | 3.9  |
| 60  | N4    | 66   | GLU  | 3.9  |
| 3   | S1    | 54   | LEU  | 3.9  |
| 3   | S1    | 184  | LEU  | 3.9  |
| 13  | C1    | 150  | ASN  | 3.9  |
| 43  | l6    | 8    | LYS  | 3.9  |
| 13  | c1    | 117  | VAL  | 3.9  |
| 21  | c9    | 17   | ALA  | 3.9  |
| 27  | d5    | 87   | GLY  | 3.9  |
| 53  | M7    | 157  | VAL  | 3.9  |
| 17  | C5    | 10   | ARG  | 3.9  |
| 47  | M0    | 221  | ALA  | 3.9  |
| 14  | c2    | 21   | GLU  | 3.9  |
| 60  | n4    | 108  | LYS  | 3.9  |
| 17  | c5    | 6    | ASN  | 3.9  |
| 1   | 6     | 660  | G    | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 71  | O5    | 120  | ALA  | 3.9  |
| 82  | p0    | 216  | ALA  | 3.9  |
| 36  | 1     | 3154 | C    | 3.9  |
| 39  | l2    | 252  | THR  | 3.9  |
| 80  | e0    | 49   | LEU  | 3.8  |
| 35  | SM    | 14   | ASP  | 3.8  |
| 82  | p0    | 203  | ASP  | 3.8  |
| 36  | 5     | 1764 | U    | 3.8  |
| 22  | d0    | 100  | VAL  | 3.8  |
| 18  | c6    | 142  | TYR  | 3.8  |
| 7   | s5    | 36   | ALA  | 3.8  |
| 36  | 5     | 439  | C    | 3.8  |
| 1   | 2     | 719  | U    | 3.8  |
| 17  | c5    | 11   | VAL  | 3.8  |
| 36  | 1     | 2397 | A    | 3.8  |
| 36  | 1     | 3155 | U    | 3.8  |
| 28  | D6    | 85   | ARG  | 3.8  |
| 13  | C1    | 151  | LYS  | 3.8  |
| 40  | l3    | 140  | ASP  | 3.8  |
| 1   | 2     | 194  | U    | 3.8  |
| 36  | 1     | 252  | U    | 3.8  |
| 36  | 5     | 3275 | U    | 3.8  |
| 5   | S3    | 43   | PRO  | 3.8  |
| 35  | SM    | 10   | ASN  | 3.8  |
| 5   | S3    | 88   | ALA  | 3.8  |
| 27  | D5    | 36   | ALA  | 3.8  |
| 41  | l4    | 63   | GLU  | 3.8  |
| 34  | sR    | 167  | VAL  | 3.8  |
| 2   | S0    | 170  | ILE  | 3.8  |
| 9   | S7    | 8    | ILE  | 3.8  |
| 45  | l8    | 254  | ASP  | 3.8  |
| 36  | 5     | 3154 | C    | 3.8  |
| 7   | s5    | 154  | ALA  | 3.8  |
| 9   | s7    | 52   | ALA  | 3.8  |
| 8   | s6    | 216  | LEU  | 3.8  |
| 18  | c6    | 2    | SER  | 3.7  |
| 19  | c7    | 88   | VAL  | 3.7  |
| 12  | c0    | 97   | PRO  | 3.7  |
| 68  | o2    | 127  | ALA  | 3.7  |
| 1   | 6     | 679  | U    | 3.7  |
| 36  | 5     | 437  | G    | 3.7  |
| 41  | L4    | 68   | GLY  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 5     | 1103 | A    | 3.7  |
| 82  | p0    | 219  | THR  | 3.7  |
| 60  | N4    | 71   | ARG  | 3.7  |
| 55  | M9    | 177  | VAL  | 3.7  |
| 5   | S3    | 217  | ILE  | 3.7  |
| 19  | c7    | 90   | ALA  | 3.7  |
| 34  | sR    | 2    | ALA  | 3.7  |
| 2   | S0    | 204  | TYR  | 3.7  |
| 1   | 6     | 320  | U    | 3.7  |
| 38  | 4     | 82   | U    | 3.7  |
| 17  | c5    | 135  | THR  | 3.7  |
| 36  | 5     | 3276 | G    | 3.7  |
| 32  | E0    | 50   | VAL  | 3.7  |
| 38  | 8     | 79   | A    | 3.7  |
| 38  | 8     | 80   | A    | 3.7  |
| 60  | N4    | 97   | LYS  | 3.7  |
| 19  | C7    | 96   | SER  | 3.7  |
| 47  | M0    | 218  | ALA  | 3.7  |
| 58  | N2    | 89   | LEU  | 3.7  |
| 16  | C4    | 41   | ARG  | 3.7  |
| 36  | 1     | 1567 | U    | 3.7  |
| 35  | SM    | 13   | GLU  | 3.7  |
| 53  | M7    | 162  | GLU  | 3.7  |
| 60  | N4    | 70   | LYS  | 3.7  |
| 65  | N9    | 25   | LYS  | 3.7  |
| 1   | 6     | 1711 | C    | 3.7  |
| 1   | 6     | 677  | G    | 3.7  |
| 17  | c5    | 136  | SER  | 3.7  |
| 8   | S6    | 124  | LEU  | 3.7  |
| 47  | M0    | 219  | ALA  | 3.7  |
| 33  | E1    | 85   | TYR  | 3.7  |
| 36  | 5     | 1351 | U    | 3.7  |
| 36  | 5     | 1016 | C    | 3.6  |
| 9   | S7    | 108  | GLN  | 3.6  |
| 34  | sR    | 162  | ALA  | 3.6  |
| 18  | c6    | 114  | ARG  | 3.6  |
| 36  | 1     | 3156 | U    | 3.6  |
| 22  | d0    | 95   | ALA  | 3.6  |
| 36  | 1     | 1762 | C    | 3.6  |
| 1   | 2     | 793  | A    | 3.6  |
| 1   | 6     | 1371 | A    | 3.6  |
| 1   | 6     | 1707 | A    | 3.6  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 52         | M6           | 80         | PHE         | 3.6         |
| 7          | S5           | 209        | TYR         | 3.6         |
| 1          | 2            | 656        | G           | 3.6         |
| 36         | 5            | 3155       | U           | 3.6         |
| 82         | p0           | 209        | LEU         | 3.6         |
| 13         | C1           | 154        | ALA         | 3.6         |
| 55         | m9           | 183        | ALA         | 3.6         |
| 19         | C7           | 125        | SER         | 3.6         |
| 1          | 2            | 658        | C           | 3.6         |
| 1          | 6            | 1399       | C           | 3.6         |
| 36         | 5            | 2256       | A           | 3.6         |
| 35         | SM           | 12         | VAL         | 3.6         |
| 58         | N2           | 108        | TYR         | 3.6         |
| 8          | S6           | 163        | THR         | 3.6         |
| 9          | s7           | 34         | LEU         | 3.6         |
| 27         | d5           | 75         | LEU         | 3.6         |
| 34         | sR           | 121        | MET         | 3.6         |
| 33         | E1           | 124        | PRO         | 3.6         |
| 1          | 2            | 558        | U           | 3.6         |
| 36         | 1            | 1095       | U           | 3.6         |
| 36         | 5            | 249        | U           | 3.6         |
| 5          | S3           | 179        | GLN         | 3.6         |
| 61         | n5           | 23         | ALA         | 3.6         |
| 67         | O1           | 79         | ARG         | 3.6         |
| 2          | S0           | 7          | PHE         | 3.6         |
| 36         | 5            | 1581       | C           | 3.6         |
| 3          | S1           | 47         | LEU         | 3.6         |
| 4          | S2           | 90         | THR         | 3.6         |
| 17         | c5           | 9          | LYS         | 3.5         |
| 13         | C1           | 149        | ALA         | 3.5         |
| 60         | N4           | 78         | ALA         | 3.5         |
| 60         | n4           | 131        | ALA         | 3.5         |
| 36         | 5            | 981        | U           | 3.5         |
| 13         | C1           | 153        | PHE         | 3.5         |
| 36         | 1            | 2095       | G           | 3.5         |
| 9          | S7           | 187        | SER         | 3.5         |
| 14         | c2           | 59         | LEU         | 3.5         |
| 2          | s0           | 204        | TYR         | 3.5         |
| 1          | 6            | 1709       | C           | 3.5         |
| 36         | 1            | 1951       | C           | 3.5         |
| 36         | 5            | 440        | A           | 3.5         |
| 9          | S7           | 12         | ALA         | 3.5         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | c1    | 147  | ALA  | 3.5  |
| 18  | c6    | 3    | ALA  | 3.5  |
| 50  | M4    | 138  | ALA  | 3.5  |
| 53  | M7    | 158  | ALA  | 3.5  |
| 8   | S6    | 226  | ILE  | 3.5  |
| 19  | c7    | 120  | SER  | 3.5  |
| 35  | SM    | 19   | VAL  | 3.5  |
| 67  | O1    | 82   | GLU  | 3.5  |
| 3   | S1    | 217  | LEU  | 3.5  |
| 18  | C6    | 57   | LEU  | 3.5  |
| 46  | L9    | 191  | LEU  | 3.5  |
| 5   | S3    | 87   | TYR  | 3.5  |
| 32  | E0    | 48   | THR  | 3.5  |
| 2   | S0    | 40   | ALA  | 3.5  |
| 9   | S7    | 6    | ALA  | 3.5  |
| 1   | 6     | 1706 | C    | 3.5  |
| 36  | 1     | 2208 | A    | 3.5  |
| 1   | 6     | 680  | U    | 3.5  |
| 36  | 5     | 2538 | U    | 3.5  |
| 39  | l2    | 213  | GLY  | 3.5  |
| 2   | S0    | 189  | VAL  | 3.5  |
| 30  | D8    | 57   | MET  | 3.5  |
| 19  | C7    | 115  | LEU  | 3.5  |
| 2   | S0    | 97   | PRO  | 3.5  |
| 2   | S0    | 206  | ASP  | 3.5  |
| 14  | c2    | 20   | ALA  | 3.5  |
| 16  | c4    | 60   | ALA  | 3.5  |
| 9   | s7    | 8    | ILE  | 3.5  |
| 1   | 2     | 715  | U    | 3.5  |
| 55  | m9    | 153  | LYS  | 3.5  |
| 60  | n4    | 73   | ARG  | 3.5  |
| 22  | d0    | 104  | THR  | 3.5  |
| 60  | n4    | 121  | ALA  | 3.5  |
| 65  | N9    | 2    | ALA  | 3.5  |
| 78  | Q2    | 106  | PHE  | 3.4  |
| 8   | S6    | 33   | GLY  | 3.4  |
| 16  | c4    | 62   | LEU  | 3.4  |
| 35  | sM    | 84   | LYS  | 3.4  |
| 1   | 2     | 239  | C    | 3.4  |
| 36  | 5     | 1569 | U    | 3.4  |
| 37  | 3     | 73   | C    | 3.4  |
| 50  | M4    | 5    | SER  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 59  | N3    | 2    | SER  | 3.4  |
| 82  | p0    | 215  | SER  | 3.4  |
| 14  | C2    | 130  | THR  | 3.4  |
| 34  | sR    | 250  | TYR  | 3.4  |
| 50  | M4    | 9    | ALA  | 3.4  |
| 60  | N4    | 90   | ILE  | 3.4  |
| 19  | c7    | 98   | GLY  | 3.4  |
| 53  | M7    | 159  | LYS  | 3.4  |
| 60  | N4    | 87   | LEU  | 3.4  |
| 60  | n4    | 71   | ARG  | 3.4  |
| 1   | 6     | 132  | U    | 3.4  |
| 36  | 1     | 1764 | U    | 3.4  |
| 1   | 2     | 135  | A    | 3.4  |
| 1   | 6     | 1701 | A    | 3.4  |
| 35  | SM    | 165  | LYS  | 3.4  |
| 7   | s5    | 150  | GLY  | 3.4  |
| 55  | M9    | 184  | LEU  | 3.4  |
| 19  | c7    | 118  | PRO  | 3.4  |
| 8   | S6    | 148  | SER  | 3.4  |
| 1   | 6     | 506  | A    | 3.4  |
| 10  | S8    | 148  | ALA  | 3.4  |
| 31  | d9    | 7    | TRP  | 3.4  |
| 35  | sM    | 82   | THR  | 3.4  |
| 1   | 2     | 500  | C    | 3.4  |
| 5   | S3    | 148  | LYS  | 3.4  |
| 8   | S6    | 171  | LYS  | 3.4  |
| 11  | S9    | 29   | LYS  | 3.4  |
| 19  | c7    | 62   | GLN  | 3.4  |
| 60  | n4    | 74   | LYS  | 3.4  |
| 32  | E0    | 49   | LEU  | 3.4  |
| 82  | p0    | 93   | LEU  | 3.4  |
| 1   | 6     | 718  | U    | 3.4  |
| 1   | 2     | 321  | C    | 3.3  |
| 59  | n3    | 3    | GLY  | 3.3  |
| 62  | N6    | 127  | GLU  | 3.3  |
| 9   | S7    | 4    | PRO  | 3.3  |
| 3   | S1    | 230  | ALA  | 3.3  |
| 22  | D0    | 106  | ILE  | 3.3  |
| 27  | D5    | 41   | ILE  | 3.3  |
| 45  | l8    | 117  | ALA  | 3.3  |
| 1   | 2     | 718  | U    | 3.3  |
| 36  | 5     | 1356 | U    | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | E1    | 103  | LEU  | 3.3  |
| 16  | C4    | 67   | VAL  | 3.3  |
| 3   | S1    | 233  | GLY  | 3.3  |
| 15  | c3    | 106  | ARG  | 3.3  |
| 36  | 5     | 2398 | A    | 3.3  |
| 1   | 6     | 136  | C    | 3.3  |
| 1   | 2     | 488  | G    | 3.3  |
| 36  | 5     | 1576 | G    | 3.3  |
| 60  | N4    | 74   | LYS  | 3.3  |
| 30  | d8    | 63   | ALA  | 3.3  |
| 82  | p0    | 221  | ALA  | 3.3  |
| 3   | s1    | 217  | LEU  | 3.3  |
| 20  | c8    | 17   | LEU  | 3.3  |
| 23  | D1    | 69   | LEU  | 3.3  |
| 66  | O0    | 104  | LEU  | 3.3  |
| 36  | 5     | 1353 | U    | 3.3  |
| 7   | S5    | 150  | GLY  | 3.3  |
| 36  | 1     | 1103 | A    | 3.3  |
| 36  | 5     | 2397 | A    | 3.3  |
| 53  | M7    | 163  | LYS  | 3.3  |
| 9   | s7    | 6    | ALA  | 3.3  |
| 22  | D0    | 99   | ILE  | 3.3  |
| 36  | 5     | 2507 | C    | 3.3  |
| 28  | D6    | 63   | ALA  | 3.3  |
| 44  | L7    | 23   | ALA  | 3.3  |
| 70  | O4    | 2    | ALA  | 3.3  |
| 8   | S6    | 67   | VAL  | 3.3  |
| 82  | p0    | 205  | THR  | 3.3  |
| 19  | c7    | 103  | ASP  | 3.3  |
| 1   | 6     | 754  | A    | 3.3  |
| 1   | 6     | 1081 | A    | 3.3  |
| 22  | d0    | 119  | ALA  | 3.3  |
| 55  | m9    | 185  | LEU  | 3.3  |
| 1   | 6     | 1082 | C    | 3.3  |
| 60  | N4    | 80   | ARG  | 3.3  |
| 16  | C4    | 48   | VAL  | 3.3  |
| 8   | S6    | 168  | THR  | 3.3  |
| 1   | 6     | 75   | U    | 3.2  |
| 26  | d4    | 99   | LYS  | 3.2  |
| 33  | e1    | 124  | PRO  | 3.2  |
| 19  | c7    | 122  | ILE  | 3.2  |
| 60  | n4    | 122  | ALA  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | C2           | 88         | LEU         | 3.2         |
| 4          | S2           | 250        | GLN         | 3.2         |
| 16         | c4           | 48         | VAL         | 3.2         |
| 2          | S0           | 44         | GLY         | 3.2         |
| 16         | C4           | 34         | SER         | 3.2         |
| 21         | C9           | 5          | SER         | 3.2         |
| 14         | C2           | 107        | ASP         | 3.2         |
| 1          | 2            | 261        | U           | 3.2         |
| 22         | D0           | 121        | ASN         | 3.2         |
| 36         | 5            | 182        | U           | 3.2         |
| 36         | 5            | 1953       | G           | 3.2         |
| 82         | p0           | 201        | ILE         | 3.2         |
| 18         | c6           | 57         | LEU         | 3.2         |
| 33         | e1           | 103        | LEU         | 3.2         |
| 35         | SM           | 15         | ALA         | 3.2         |
| 60         | N4           | 85         | ALA         | 3.2         |
| 12         | c0           | 95         | ARG         | 3.2         |
| 32         | E0           | 54         | ARG         | 3.2         |
| 40         | l3           | 146        | ARG         | 3.2         |
| 34         | sR           | 61         | PHE         | 3.2         |
| 18         | c6           | 19         | VAL         | 3.2         |
| 1          | 2            | 369        | A           | 3.2         |
| 35         | SM           | 83         | LYS         | 3.2         |
| 36         | 5            | 1580       | A           | 3.2         |
| 2          | s0           | 186        | GLY         | 3.2         |
| 34         | sR           | 317        | THR         | 3.2         |
| 59         | N3           | 3          | GLY         | 3.2         |
| 1          | 6            | 659        | C           | 3.2         |
| 12         | C0           | 91         | TYR         | 3.2         |
| 30         | D8           | 21         | SER         | 3.2         |
| 36         | 1            | 1579       | C           | 3.2         |
| 22         | d0           | 99         | ILE         | 3.2         |
| 82         | p0           | 206        | ASP         | 3.2         |
| 12         | c0           | 96         | ASN         | 3.2         |
| 19         | C7           | 73         | LEU         | 3.2         |
| 34         | sR           | 284        | ALA         | 3.2         |
| 35         | sM           | 155        | LEU         | 3.2         |
| 10         | s8           | 195        | ARG         | 3.2         |
| 33         | E1           | 145        | HIS         | 3.2         |
| 33         | e1           | 145        | HIS         | 3.2         |
| 1          | 2            | 714        | G           | 3.2         |
| 1          | 6            | 656        | G           | 3.2         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 6     | 1696 | G    | 3.2  |
| 8   | S6    | 164  | LYS  | 3.2  |
| 7   | S5    | 151  | GLY  | 3.2  |
| 1   | 2     | 541  | A    | 3.2  |
| 30  | d8    | 65   | ARG  | 3.2  |
| 35  | sM    | 156  | ASN  | 3.2  |
| 1   | 2     | 792  | U    | 3.2  |
| 1   | 6     | 1060 | U    | 3.2  |
| 2   | S0    | 102  | PHE  | 3.2  |
| 22  | d0    | 105  | GLN  | 3.2  |
| 1   | 6     | 651  | G    | 3.2  |
| 8   | S6    | 66   | GLY  | 3.2  |
| 60  | n4    | 64   | THR  | 3.2  |
| 22  | d0    | 19   | ILE  | 3.2  |
| 36  | 5     | 1355 | A    | 3.1  |
| 8   | s6    | 217  | SER  | 3.1  |
| 29  | D7    | 41   | LEU  | 3.1  |
| 2   | S0    | 5    | ALA  | 3.1  |
| 28  | d6    | 47   | ALA  | 3.1  |
| 60  | n4    | 110  | LYS  | 3.1  |
| 4   | S2    | 93   | GLY  | 3.1  |
| 60  | n4    | 75   | THR  | 3.1  |
| 14  | c2    | 136  | ILE  | 3.1  |
| 65  | N9    | 24   | PRO  | 3.1  |
| 1   | 2     | 279  | G    | 3.1  |
| 4   | s2    | 91   | ARG  | 3.1  |
| 40  | l3    | 387  | LEU  | 3.1  |
| 14  | C2    | 20   | ALA  | 3.1  |
| 53  | M7    | 160  | ALA  | 3.1  |
| 1   | 6     | 1712 | A    | 3.1  |
| 14  | c2    | 22   | VAL  | 3.1  |
| 19  | c7    | 99   | VAL  | 3.1  |
| 1   | 2     | 697  | C    | 3.1  |
| 1   | 2     | 716  | C    | 3.1  |
| 8   | S6    | 225  | GLU  | 3.1  |
| 34  | SR    | 160  | GLU  | 3.1  |
| 5   | s3    | 216  | PRO  | 3.1  |
| 19  | C7    | 86   | PRO  | 3.1  |
| 17  | C5    | 8    | LYS  | 3.1  |
| 9   | S7    | 52   | ALA  | 3.1  |
| 30  | D8    | 7    | VAL  | 3.1  |
| 36  | 1     | 2971 | A    | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 82  | p0    | 208  | GLU  | 3.1  |
| 6   | s4    | 261  | LEU  | 3.1  |
| 12  | c0    | 2    | LEU  | 3.1  |
| 35  | sM    | 83   | LYS  | 3.1  |
| 11  | S9    | 181  | ALA  | 3.1  |
| 28  | D6    | 47   | ALA  | 3.1  |
| 72  | o6    | 100  | HIS  | 3.1  |
| 2   | s0    | 206  | ASP  | 3.1  |
| 46  | l9    | 190  | ASP  | 3.1  |
| 60  | n4    | 130  | SER  | 3.1  |
| 82  | p0    | 199  | SER  | 3.1  |
| 60  | n4    | 84   | GLY  | 3.1  |
| 1   | 6     | 579  | A    | 3.1  |
| 36  | 1     | 981  | U    | 3.1  |
| 9   | s7    | 58   | LEU  | 3.1  |
| 30  | D8    | 9    | LEU  | 3.1  |
| 43  | L6    | 129  | GLU  | 3.1  |
| 16  | C4    | 119  | THR  | 3.1  |
| 25  | D3    | 3    | LYS  | 3.1  |
| 65  | n9    | 25   | LYS  | 3.1  |
| 67  | O1    | 4    | LEU  | 3.1  |
| 44  | l7    | 22   | THR  | 3.1  |
| 3   | S1    | 24   | PHE  | 3.0  |
| 19  | C7    | 89   | SER  | 3.0  |
| 47  | m0    | 220  | GLN  | 3.0  |
| 69  | o3    | 107  | ILE  | 3.0  |
| 10  | S8    | 200  | LYS  | 3.0  |
| 17  | c5    | 8    | LYS  | 3.0  |
| 26  | d4    | 127  | LYS  | 3.0  |
| 1   | 2     | 280  | U    | 3.0  |
| 9   | s7    | 32   | PRO  | 3.0  |
| 65  | n9    | 24   | PRO  | 3.0  |
| 1   | 2     | 505  | A    | 3.0  |
| 1   | 2     | 1371 | A    | 3.0  |
| 8   | s6    | 168  | THR  | 3.0  |
| 60  | n4    | 83   | THR  | 3.0  |
| 1   | 2     | 676  | G    | 3.0  |
| 1   | 6     | 720  | G    | 3.0  |
| 2   | s0    | 5    | ALA  | 3.0  |
| 7   | S5    | 24   | VAL  | 3.0  |
| 8   | S6    | 41   | VAL  | 3.0  |
| 1   | 2     | 1399 | C    | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | 1            | 1556       | C           | 3.0         |
| 34         | SR           | 52         | GLN         | 3.0         |
| 47         | m0           | 112        | GLN         | 3.0         |
| 80         | e0           | 63         | GLN         | 3.0         |
| 6          | S4           | 254        | ARG         | 3.0         |
| 30         | d8           | 64         | ARG         | 3.0         |
| 65         | N9           | 59         | LYS         | 3.0         |
| 35         | SM           | 21         | PRO         | 3.0         |
| 1          | 6            | 194        | U           | 3.0         |
| 3          | S1           | 46         | THR         | 3.0         |
| 1          | 6            | 1694       | A           | 3.0         |
| 36         | 1            | 2398       | A           | 3.0         |
| 68         | O2           | 127        | ALA         | 3.0         |
| 3          | S1           | 223        | PHE         | 3.0         |
| 3          | s1           | 20         | VAL         | 3.0         |
| 16         | C4           | 29         | HIS         | 3.0         |
| 20         | c8           | 4          | VAL         | 3.0         |
| 33         | E1           | 150        | VAL         | 3.0         |
| 3          | S1           | 55         | LYS         | 3.0         |
| 36         | 5            | 1192       | C           | 3.0         |
| 45         | l8           | 123        | GLN         | 3.0         |
| 66         | o0           | 100        | ILE         | 3.0         |
| 2          | S0           | 28         | ASN         | 3.0         |
| 10         | S8           | 193        | LEU         | 3.0         |
| 11         | S9           | 116        | LEU         | 3.0         |
| 16         | C4           | 66         | ASP         | 3.0         |
| 8          | s6           | 166        | GLU         | 3.0         |
| 12         | c0           | 90         | THR         | 3.0         |
| 1          | 6            | 681        | U           | 3.0         |
| 10         | S8           | 106        | ALA         | 3.0         |
| 18         | C6           | 20         | ALA         | 3.0         |
| 36         | 1            | 2996       | U           | 3.0         |
| 82         | p0           | 106        | ALA         | 3.0         |
| 14         | c2           | 86         | VAL         | 3.0         |
| 2          | S0           | 110        | TYR         | 3.0         |
| 2          | s0           | 110        | TYR         | 3.0         |
| 2          | S0           | 166        | GLY         | 3.0         |
| 3          | S1           | 63         | GLY         | 3.0         |
| 13         | C1           | 5          | LEU         | 3.0         |
| 19         | C7           | 74         | GLN         | 3.0         |
| 30         | d8           | 24         | GLY         | 3.0         |
| 36         | 5            | 443        | G           | 3.0         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | c9    | 2    | PRO  | 3.0  |
| 30  | d8    | 39   | THR  | 3.0  |
| 34  | SR    | 162  | ALA  | 3.0  |
| 56  | N0    | 2    | ALA  | 3.0  |
| 28  | D6    | 58   | VAL  | 3.0  |
| 1   | 2     | 137  | U    | 3.0  |
| 10  | s8    | 199  | LYS  | 2.9  |
| 19  | C7    | 72   | LYS  | 2.9  |
| 36  | 5     | 980  | A    | 2.9  |
| 48  | m1    | 116  | TYR  | 2.9  |
| 4   | S2    | 75   | GLY  | 2.9  |
| 39  | L2    | 13   | GLY  | 2.9  |
| 67  | o1    | 4    | LEU  | 2.9  |
| 35  | SM    | 167  | PRO  | 2.9  |
| 60  | n4    | 135  | SER  | 2.9  |
| 1   | 6     | 1695 | G    | 2.9  |
| 14  | c2    | 128  | ALA  | 2.9  |
| 34  | sR    | 279  | ALA  | 2.9  |
| 6   | S4    | 159  | THR  | 2.9  |
| 22  | d0    | 118  | VAL  | 2.9  |
| 34  | sR    | 186  | PHE  | 2.9  |
| 10  | s8    | 123  | LYS  | 2.9  |
| 22  | D0    | 21   | LYS  | 2.9  |
| 36  | 1     | 1572 | U    | 2.9  |
| 36  | 5     | 2979 | U    | 2.9  |
| 14  | c2    | 106  | ILE  | 2.9  |
| 58  | N2    | 41   | ILE  | 2.9  |
| 60  | n4    | 132  | GLY  | 2.9  |
| 58  | n2    | 52   | ASN  | 2.9  |
| 59  | n3    | 4    | ASN  | 2.9  |
| 57  | N1    | 126  | VAL  | 2.9  |
| 60  | N4    | 64   | THR  | 2.9  |
| 66  | o0    | 32   | LYS  | 2.9  |
| 1   | 6     | 1634 | C    | 2.9  |
| 72  | O6    | 56   | ARG  | 2.9  |
| 36  | 1     | 494  | G    | 2.9  |
| 48  | m1    | 65   | ILE  | 2.9  |
| 1   | 2     | 1362 | U    | 2.9  |
| 9   | S7    | 41   | LEU  | 2.9  |
| 19  | C7    | 119  | LEU  | 2.9  |
| 38  | 4     | 81   | U    | 2.9  |
| 22  | D0    | 17   | GLN  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | SR    | 79   | TYR  | 2.9  |
| 12  | c0    | 83   | PRO  | 2.9  |
| 17  | C5    | 53   | PRO  | 2.9  |
| 45  | L8    | 240  | ASN  | 2.9  |
| 8   | s6    | 162  | VAL  | 2.9  |
| 9   | S7    | 20   | VAL  | 2.9  |
| 17  | C5    | 9    | LYS  | 2.9  |
| 47  | m0    | 195  | ALA  | 2.9  |
| 8   | S6    | 156  | PHE  | 2.9  |
| 4   | s2    | 96   | THR  | 2.9  |
| 5   | s3    | 44   | THR  | 2.9  |
| 28  | d6    | 10   | ARG  | 2.9  |
| 2   | s0    | 173  | ILE  | 2.9  |
| 58  | N2    | 11   | ILE  | 2.9  |
| 3   | S1    | 96   | LEU  | 2.9  |
| 22  | D0    | 93   | LEU  | 2.9  |
| 4   | s2    | 93   | GLY  | 2.9  |
| 36  | 1     | 2539 | C    | 2.9  |
| 36  | 1     | 3287 | U    | 2.9  |
| 9   | S7    | 32   | PRO  | 2.9  |
| 49  | m3    | 133  | PRO  | 2.9  |
| 65  | n9    | 27   | TYR  | 2.9  |
| 67  | o1    | 82   | GLU  | 2.9  |
| 27  | D5    | 97   | LYS  | 2.9  |
| 60  | n4    | 117  | LYS  | 2.9  |
| 35  | SM    | 160  | ASN  | 2.9  |
| 35  | sM    | 164  | ASN  | 2.9  |
| 3   | S1    | 60   | ALA  | 2.9  |
| 3   | S1    | 65   | VAL  | 2.9  |
| 47  | m0    | 2    | ALA  | 2.9  |
| 38  | 4     | 80   | A    | 2.9  |
| 55  | M9    | 104  | ARG  | 2.9  |
| 69  | o3    | 60   | ARG  | 2.9  |
| 7   | s5    | 42   | LEU  | 2.9  |
| 12  | C0    | 92   | ILE  | 2.9  |
| 27  | D5    | 69   | LEU  | 2.9  |
| 66  | o0    | 104  | LEU  | 2.9  |
| 1   | 2     | 1370 | U    | 2.8  |
| 1   | 6     | 493  | U    | 2.8  |
| 1   | 6     | 719  | U    | 2.8  |
| 27  | d5    | 46   | LYS  | 2.8  |
| 33  | e1    | 85   | TYR  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 6     | 1698 | G    | 2.8  |
| 3   | S1    | 225  | VAL  | 2.8  |
| 26  | D4    | 100  | VAL  | 2.8  |
| 10  | S8    | 195  | ARG  | 2.8  |
| 15  | c3    | 15   | ALA  | 2.8  |
| 52  | M6    | 3    | VAL  | 2.8  |
| 22  | d0    | 121  | ASN  | 2.8  |
| 27  | D5    | 82   | HIS  | 2.8  |
| 45  | l8    | 121  | SER  | 2.8  |
| 72  | O6    | 100  | HIS  | 2.8  |
| 14  | C2    | 24   | ILE  | 2.8  |
| 19  | C7    | 100  | LEU  | 2.8  |
| 34  | sR    | 141  | LEU  | 2.8  |
| 82  | p0    | 100  | ILE  | 2.8  |
| 10  | S8    | 135  | LYS  | 2.8  |
| 26  | D4    | 128  | LYS  | 2.8  |
| 43  | l6    | 9    | TRP  | 2.8  |
| 18  | C6    | 92   | TYR  | 2.8  |
| 1   | 2     | 233  | C    | 2.8  |
| 18  | c6    | 143  | ARG  | 2.8  |
| 28  | d6    | 58   | VAL  | 2.8  |
| 33  | E1    | 152  | ALA  | 2.8  |
| 36  | 5     | 1017 | C    | 2.8  |
| 38  | 8     | 83   | C    | 2.8  |
| 18  | C6    | 29   | ILE  | 2.8  |
| 18  | c6    | 29   | ILE  | 2.8  |
| 68  | O2    | 26   | HIS  | 2.8  |
| 2   | S0    | 6    | THR  | 2.8  |
| 2   | s0    | 2    | SER  | 2.8  |
| 8   | s6    | 163  | THR  | 2.8  |
| 29  | d7    | 58   | SER  | 2.8  |
| 35  | sM    | 85   | SER  | 2.8  |
| 36  | 1     | 1576 | G    | 2.8  |
| 41  | L4    | 67   | THR  | 2.8  |
| 1   | 2     | 1151 | A    | 2.8  |
| 60  | n4    | 115  | LYS  | 2.8  |
| 2   | s0    | 194  | PRO  | 2.8  |
| 17  | C5    | 104  | GLN  | 2.8  |
| 30  | d8    | 6    | PRO  | 2.8  |
| 82  | p0    | 78   | PRO  | 2.8  |
| 29  | D7    | 75   | GLU  | 2.8  |
| 1   | 6     | 665  | U    | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | s0    | 189  | VAL  | 2.8  |
| 5   | s3    | 225  | TYR  | 2.8  |
| 7   | s5    | 156  | ARG  | 2.8  |
| 16  | c4    | 67   | VAL  | 2.8  |
| 42  | l5    | 272  | TYR  | 2.8  |
| 27  | d5    | 104  | ALA  | 2.8  |
| 36  | 5     | 1094 | U    | 2.8  |
| 7   | s5    | 43   | PHE  | 2.8  |
| 3   | S1    | 32   | ILE  | 2.8  |
| 8   | S6    | 73   | ILE  | 2.8  |
| 27  | D5    | 38   | HIS  | 2.8  |
| 60  | n4    | 63   | ILE  | 2.8  |
| 13  | C1    | 155  | LYS  | 2.8  |
| 55  | M9    | 180  | LYS  | 2.8  |
| 9   | S7    | 53   | GLY  | 2.8  |
| 2   | s0    | 193  | GLN  | 2.8  |
| 36  | 1     | 2418 | G    | 2.8  |
| 12  | C0    | 95   | ARG  | 2.8  |
| 20  | c8    | 5    | VAL  | 2.8  |
| 82  | p0    | 188  | VAL  | 2.8  |
| 9   | s7    | 24   | PHE  | 2.8  |
| 34  | SR    | 180  | ALA  | 2.8  |
| 1   | 2     | 73   | U    | 2.8  |
| 1   | 2     | 1363 | U    | 2.8  |
| 1   | 6     | 494  | U    | 2.8  |
| 8   | S6    | 158  | ILE  | 2.8  |
| 10  | s8    | 183  | ILE  | 2.8  |
| 14  | C2    | 136  | ILE  | 2.8  |
| 34  | SR    | 115  | ILE  | 2.8  |
| 55  | m9    | 184  | LEU  | 2.8  |
| 69  | o3    | 87   | ASN  | 2.8  |
| 10  | S8    | 199  | LYS  | 2.8  |
| 26  | d4    | 128  | LYS  | 2.8  |
| 33  | e1    | 87   | THR  | 2.8  |
| 1   | 2     | 1637 | C    | 2.8  |
| 1   | 6     | 239  | C    | 2.8  |
| 1   | 6     | 1705 | C    | 2.8  |
| 2   | S0    | 128  | SER  | 2.8  |
| 7   | S5    | 153  | GLY  | 2.8  |
| 1   | 2     | 754  | A    | 2.7  |
| 1   | 6     | 661  | A    | 2.7  |
| 1   | 6     | 793  | A    | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | L5    | 185  | PHE  | 2.7  |
| 49  | m3    | 191  | ALA  | 2.7  |
| 1   | 6     | 1690 | G    | 2.7  |
| 82  | p0    | 213  | PHE  | 2.7  |
| 22  | D0    | 20   | ILE  | 2.7  |
| 82  | p0    | 204  | ILE  | 2.7  |
| 1   | 6     | 1708 | U    | 2.7  |
| 14  | C2    | 111  | ASN  | 2.7  |
| 7   | s5    | 225  | ARG  | 2.7  |
| 18  | C6    | 114  | ARG  | 2.7  |
| 26  | d4    | 106  | GLN  | 2.7  |
| 69  | O3    | 60   | ARG  | 2.7  |
| 36  | 5     | 175  | C    | 2.7  |
| 36  | 5     | 1562 | C    | 2.7  |
| 62  | n6    | 127  | GLU  | 2.7  |
| 20  | C8    | 22   | VAL  | 2.7  |
| 5   | S3    | 107  | PHE  | 2.7  |
| 5   | s3    | 69   | LEU  | 2.7  |
| 5   | s3    | 145  | ALA  | 2.7  |
| 44  | l7    | 27   | ALA  | 2.7  |
| 49  | M3    | 193  | ALA  | 2.7  |
| 49  | m3    | 132  | ALA  | 2.7  |
| 58  | N2    | 12   | ALA  | 2.7  |
| 7   | S5    | 137  | ILE  | 2.7  |
| 3   | S1    | 45   | LYS  | 2.7  |
| 14  | C2    | 137  | MET  | 2.7  |
| 36  | 1     | 2100 | A    | 2.7  |
| 36  | 1     | 2540 | A    | 2.7  |
| 1   | 2     | 132  | U    | 2.7  |
| 1   | 6     | 137  | U    | 2.7  |
| 8   | s6    | 146  | GLY  | 2.7  |
| 60  | N4    | 94   | ARG  | 2.7  |
| 82  | p0    | 102  | SER  | 2.7  |
| 9   | s7    | 5    | GLN  | 2.7  |
| 7   | S5    | 33   | VAL  | 2.7  |
| 33  | e1    | 102  | VAL  | 2.7  |
| 1   | 2     | 1082 | C    | 2.7  |
| 2   | S0    | 203  | PHE  | 2.7  |
| 15  | c3    | 149  | LEU  | 2.7  |
| 26  | D4    | 126  | ALA  | 2.7  |
| 35  | SM    | 176  | ALA  | 2.7  |
| 41  | l4    | 352  | ALA  | 2.7  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | S1    | 29   | TRP  | 2.7  |
| 8   | S6    | 169  | TYR  | 2.7  |
| 18  | C6    | 96   | TYR  | 2.7  |
| 1   | 6     | 1704 | U    | 2.7  |
| 36  | 1     | 2097 | U    | 2.7  |
| 36  | 5     | 1765 | U    | 2.7  |
| 11  | S9    | 5    | PRO  | 2.7  |
| 30  | D8    | 6    | PRO  | 2.7  |
| 70  | O4    | 16   | ARG  | 2.7  |
| 14  | c2    | 119  | SER  | 2.7  |
| 47  | M0    | 112  | GLN  | 2.7  |
| 35  | sM    | 172  | VAL  | 2.7  |
| 4   | s2    | 92   | ALA  | 2.7  |
| 19  | C7    | 71   | PHE  | 2.7  |
| 22  | D0    | 108  | ILE  | 2.7  |
| 35  | sM    | 119  | ALA  | 2.7  |
| 71  | O5    | 2    | ALA  | 2.7  |
| 71  | o5    | 2    | ALA  | 2.7  |
| 44  | l7    | 158  | LYS  | 2.7  |
| 8   | s6    | 22   | HIS  | 2.7  |
| 18  | C6    | 21   | HIS  | 2.7  |
| 1   | 6     | 658  | C    | 2.7  |
| 36  | 1     | 2772 | C    | 2.7  |
| 41  | l4    | 73   | ARG  | 2.7  |
| 48  | M1    | 55   | ARG  | 2.7  |
| 16  | C4    | 75   | GLY  | 2.7  |
| 17  | c5    | 50   | THR  | 2.7  |
| 22  | D0    | 104  | THR  | 2.7  |
| 23  | D1    | 47   | PRO  | 2.7  |
| 35  | SM    | 161  | ASN  | 2.7  |
| 36  | 1     | 979  | U    | 2.7  |
| 36  | 1     | 1950 | U    | 2.7  |
| 35  | SM    | 153  | ASP  | 2.7  |
| 67  | O1    | 6    | ASP  | 2.7  |
| 30  | D8    | 15   | VAL  | 2.7  |
| 3   | S1    | 135  | LEU  | 2.7  |
| 27  | d5    | 88   | ILE  | 2.6  |
| 66  | o0    | 6    | SER  | 2.7  |
| 8   | s6    | 164  | LYS  | 2.6  |
| 11  | S9    | 90   | LYS  | 2.6  |
| 12  | C0    | 30   | ALA  | 2.6  |
| 17  | C5    | 12   | PHE  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 60  | n4    | 97   | LYS  | 2.6  |
| 79  | Q3    | 92   | ALA  | 2.6  |
| 36  | 1     | 1577 | G    | 2.6  |
| 8   | S6    | 208  | TYR  | 2.6  |
| 30  | d8    | 61   | ARG  | 2.6  |
| 3   | S1    | 37   | THR  | 2.6  |
| 59  | N3    | 4    | ASN  | 2.6  |
| 3   | S1    | 131  | ASP  | 2.6  |
| 3   | S1    | 188  | LEU  | 2.6  |
| 8   | S6    | 21   | GLU  | 2.6  |
| 10  | s8    | 187  | GLU  | 2.6  |
| 14  | c2    | 45   | LEU  | 2.6  |
| 16  | C4    | 37   | GLU  | 2.6  |
| 34  | sR    | 51   | ASP  | 2.6  |
| 34  | sR    | 165  | ASP  | 2.6  |
| 36  | 1     | 1765 | U    | 2.6  |
| 36  | 1     | 2501 | U    | 2.6  |
| 44  | l7    | 26   | VAL  | 2.6  |
| 55  | M9    | 152  | GLU  | 2.6  |
| 58  | n2    | 11   | ILE  | 2.6  |
| 82  | p0    | 220  | ILE  | 2.6  |
| 2   | S0    | 2    | SER  | 2.6  |
| 5   | s3    | 3    | ALA  | 2.6  |
| 17  | C5    | 49   | MET  | 2.6  |
| 63  | n7    | 124  | ALA  | 2.6  |
| 1   | 2     | 730  | G    | 2.6  |
| 36  | 1     | 2400 | G    | 2.6  |
| 10  | S8    | 50   | GLY  | 2.6  |
| 17  | c5    | 132  | GLY  | 2.6  |
| 28  | D6    | 9    | GLY  | 2.6  |
| 29  | d7    | 76   | GLY  | 2.6  |
| 60  | N4    | 84   | GLY  | 2.6  |
| 64  | N8    | 33   | GLY  | 2.6  |
| 3   | S1    | 222  | LYS  | 2.6  |
| 7   | s5    | 27   | THR  | 2.6  |
| 22  | d0    | 107  | THR  | 2.6  |
| 6   | s4    | 208  | VAL  | 2.6  |
| 16  | C4    | 102  | LEU  | 2.6  |
| 20  | c8    | 15   | LEU  | 2.6  |
| 33  | e1    | 100  | LEU  | 2.6  |
| 36  | 1     | 1582 | C    | 2.6  |
| 29  | d7    | 5    | GLN  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | m9    | 187  | GLU  | 2.6  |
| 1   | 2     | 240  | U    | 2.6  |
| 1   | 2     | 1057 | U    | 2.6  |
| 1   | 6     | 721  | U    | 2.6  |
| 1   | 6     | 1398 | U    | 2.6  |
| 3   | s1    | 89   | ASP  | 2.6  |
| 35  | SM    | 163  | PHE  | 2.6  |
| 36  | 1     | 1353 | U    | 2.6  |
| 36  | 1     | 1555 | U    | 2.6  |
| 36  | 5     | 181  | U    | 2.6  |
| 36  | 5     | 620  | U    | 2.6  |
| 36  | 5     | 1763 | U    | 2.6  |
| 60  | n4    | 88   | ASP  | 2.6  |
| 13  | C1    | 144  | ALA  | 2.6  |
| 17  | C5    | 54   | ALA  | 2.6  |
| 1   | 2     | 733  | A    | 2.6  |
| 41  | L4    | 85   | SER  | 2.6  |
| 45  | L8    | 121  | SER  | 2.6  |
| 73  | O7    | 87   | SER  | 2.6  |
| 3   | S1    | 64   | ARG  | 2.6  |
| 34  | sR    | 79   | TYR  | 2.6  |
| 3   | S1    | 93   | GLY  | 2.6  |
| 28  | d6    | 98   | PRO  | 2.6  |
| 29  | D7    | 39   | GLY  | 2.6  |
| 34  | SR    | 283  | LYS  | 2.6  |
| 43  | L6    | 8    | LYS  | 2.6  |
| 45  | l8    | 122  | LYS  | 2.6  |
| 5   | S3    | 29   | LEU  | 2.6  |
| 27  | D5    | 40   | VAL  | 2.6  |
| 29  | d7    | 43   | ILE  | 2.6  |
| 60  | n4    | 76   | VAL  | 2.6  |
| 66  | o0    | 67   | VAL  | 2.6  |
| 16  | C4    | 99   | GLN  | 2.6  |
| 34  | sR    | 316  | MET  | 2.6  |
| 10  | S8    | 198  | ALA  | 2.6  |
| 14  | c2    | 92   | ALA  | 2.6  |
| 35  | SM    | 90   | ALA  | 2.6  |
| 49  | m3    | 193  | ALA  | 2.6  |
| 1   | 6     | 1490 | C    | 2.6  |
| 36  | 1     | 546  | C    | 2.6  |
| 10  | S8    | 8    | ARG  | 2.6  |
| 8   | S6    | 181  | PRO  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | c0    | 76   | LEU  | 2.6  |
| 30  | D8    | 33   | LEU  | 2.6  |
| 4   | S2    | 237  | VAL  | 2.6  |
| 22  | D0    | 100  | VAL  | 2.6  |
| 27  | D5    | 105  | THR  | 2.6  |
| 28  | D6    | 44   | ILE  | 2.6  |
| 31  | d9    | 23   | VAL  | 2.6  |
| 53  | M7    | 182  | ILE  | 2.6  |
| 19  | C7    | 83   | GLN  | 2.6  |
| 40  | L3    | 139  | GLN  | 2.6  |
| 42  | l5    | 4    | GLN  | 2.6  |
| 16  | C4    | 14   | PHE  | 2.6  |
| 45  | l8    | 114  | ALA  | 2.6  |
| 63  | n7    | 7    | ALA  | 2.6  |
| 82  | p0    | 98   | ASN  | 2.6  |
| 1   | 2     | 712  | G    | 2.5  |
| 36  | 1     | 3286 | G    | 2.5  |
| 36  | 5     | 442  | G    | 2.5  |
| 1   | 2     | 278  | U    | 2.5  |
| 7   | s5    | 148  | ARG  | 2.5  |
| 36  | 5     | 2506 | U    | 2.5  |
| 1   | 6     | 139  | C    | 2.5  |
| 36  | 1     | 2507 | C    | 2.5  |
| 36  | 5     | 1574 | C    | 2.5  |
| 4   | S2    | 34   | GLY  | 2.5  |
| 14  | C2    | 82   | PRO  | 2.5  |
| 5   | S3    | 225  | TYR  | 2.5  |
| 9   | s7    | 93   | LEU  | 2.5  |
| 34  | sR    | 32   | LEU  | 2.5  |
| 34  | sR    | 49   | GLY  | 2.5  |
| 35  | SM    | 174  | LEU  | 2.5  |
| 47  | m0    | 204  | GLY  | 2.5  |
| 82  | p0    | 202  | LEU  | 2.5  |
| 76  | q0    | 77   | ILE  | 2.5  |
| 82  | p0    | 87   | VAL  | 2.5  |
| 5   | S3    | 44   | THR  | 2.5  |
| 6   | S4    | 117  | GLU  | 2.5  |
| 35  | SM    | 152  | GLN  | 2.5  |
| 35  | SM    | 162  | GLN  | 2.5  |
| 41  | l4    | 54   | GLU  | 2.5  |
| 44  | L7    | 24   | GLU  | 2.5  |
| 60  | n4    | 133  | THR  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | E1    | 101  | ALA  | 2.5  |
| 19  | c7    | 104  | ASN  | 2.5  |
| 8   | S6    | 20   | ASP  | 2.5  |
| 13  | c1    | 116  | ARG  | 2.5  |
| 82  | p0    | 212  | HIS  | 2.5  |
| 1   | 2     | 75   | U    | 2.5  |
| 1   | 2     | 133  | U    | 2.5  |
| 35  | sM    | 170  | LYS  | 2.5  |
| 36  | 1     | 1763 | U    | 2.5  |
| 36  | 5     | 1348 | U    | 2.5  |
| 46  | l9    | 106  | LYS  | 2.5  |
| 36  | 1     | 2169 | G    | 2.5  |
| 36  | 5     | 1573 | G    | 2.5  |
| 1   | 2     | 717  | C    | 2.5  |
| 36  | 1     | 1017 | C    | 2.5  |
| 36  | 5     | 1762 | C    | 2.5  |
| 3   | S1    | 61   | LEU  | 2.5  |
| 27  | D5    | 42   | LEU  | 2.5  |
| 43  | l6    | 11   | PRO  | 2.5  |
| 4   | s2    | 86   | VAL  | 2.5  |
| 10  | S8    | 104  | ILE  | 2.5  |
| 22  | D0    | 103  | ILE  | 2.5  |
| 12  | c0    | 79   | TYR  | 2.5  |
| 34  | SR    | 8    | VAL  | 2.5  |
| 20  | C8    | 8    | GLN  | 2.5  |
| 39  | l2    | 253  | GLN  | 2.5  |
| 41  | L4    | 60   | THR  | 2.5  |
| 7   | S5    | 154  | ALA  | 2.5  |
| 7   | S5    | 155  | ALA  | 2.5  |
| 16  | c4    | 50   | ALA  | 2.5  |
| 53  | M7    | 156  | ALA  | 2.5  |
| 66  | O0    | 95   | ALA  | 2.5  |
| 70  | O4    | 111  | ALA  | 2.5  |
| 7   | S5    | 41   | LYS  | 2.5  |
| 14  | C2    | 85   | LYS  | 2.5  |
| 1   | 2     | 134  | U    | 2.5  |
| 36  | 5     | 250  | U    | 2.5  |
| 50  | m4    | 2    | SER  | 2.5  |
| 8   | S6    | 1    | MET  | 2.5  |
| 35  | sM    | 52   | PRO  | 2.5  |
| 43  | l6    | 130  | ILE  | 2.5  |
| 18  | C6    | 39   | VAL  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | D4    | 129  | VAL  | 2.5  |
| 60  | N4    | 67   | VAL  | 2.5  |
| 36  | 1     | 1574 | C    | 2.5  |
| 1   | 2     | 503  | G    | 2.5  |
| 1   | 2     | 823  | G    | 2.5  |
| 36  | 5     | 1354 | G    | 2.5  |
| 36  | 5     | 2210 | G    | 2.5  |
| 2   | S0    | 107  | PHE  | 2.5  |
| 35  | sM    | 122  | GLU  | 2.5  |
| 45  | l8    | 118  | GLU  | 2.5  |
| 67  | o1    | 83   | GLU  | 2.5  |
| 5   | S3    | 219  | ALA  | 2.5  |
| 22  | D0    | 107  | THR  | 2.5  |
| 29  | d7    | 45   | THR  | 2.5  |
| 35  | SM    | 141  | ALA  | 2.5  |
| 5   | S3    | 143  | ARG  | 2.5  |
| 15  | C3    | 138  | ASN  | 2.5  |
| 16  | c4    | 49   | LYS  | 2.5  |
| 45  | l8    | 120  | LYS  | 2.5  |
| 67  | O1    | 5    | LYS  | 2.5  |
| 70  | O4    | 113  | LYS  | 2.5  |
| 4   | S2    | 245  | ASP  | 2.5  |
| 19  | C7    | 103  | ASP  | 2.5  |
| 46  | l9    | 107  | ASP  | 2.5  |
| 3   | S1    | 207  | LEU  | 2.5  |
| 18  | c6    | 141  | SER  | 2.5  |
| 1   | 2     | 74   | U    | 2.5  |
| 19  | C7    | 38   | ILE  | 2.5  |
| 21  | C9    | 116  | ILE  | 2.5  |
| 27  | d5    | 72   | GLY  | 2.5  |
| 35  | SM    | 98   | GLY  | 2.5  |
| 36  | 1     | 1815 | U    | 2.5  |
| 36  | 5     | 2505 | U    | 2.5  |
| 49  | M3    | 130  | GLY  | 2.5  |
| 3   | S1    | 88   | VAL  | 2.5  |
| 31  | d9    | 6    | VAL  | 2.5  |
| 7   | S5    | 20   | PHE  | 2.5  |
| 8   | S6    | 222  | GLU  | 2.5  |
| 10  | s8    | 61   | GLU  | 2.5  |
| 33  | e1    | 148  | TYR  | 2.5  |
| 34  | sR    | 244  | ALA  | 2.5  |
| 35  | sM    | 158  | GLN  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | L3    | 146  | ARG  | 2.5  |
| 40  | L3    | 382  | THR  | 2.5  |
| 53  | m7    | 156  | ALA  | 2.5  |
| 55  | M9    | 151  | ARG  | 2.5  |
| 58  | N2    | 31   | ALA  | 2.5  |
| 72  | O6    | 99   | ARG  | 2.5  |
| 17  | C5    | 52   | LYS  | 2.5  |
| 33  | e1    | 79   | LYS  | 2.5  |
| 36  | 5     | 3164 | C    | 2.5  |
| 36  | 1     | 1580 | A    | 2.5  |
| 2   | s0    | 43   | ASP  | 2.4  |
| 5   | S3    | 218  | LEU  | 2.4  |
| 22  | d0    | 93   | LEU  | 2.4  |
| 48  | M1    | 28   | ASP  | 2.4  |
| 74  | O8    | 31   | LEU  | 2.4  |
| 27  | D5    | 89   | ILE  | 2.4  |
| 39  | l2    | 15   | ILE  | 2.4  |
| 3   | S1    | 178  | GLY  | 2.4  |
| 7   | S5    | 149  | VAL  | 2.4  |
| 8   | S6    | 12   | SER  | 2.4  |
| 24  | D2    | 76   | SER  | 2.4  |
| 1   | 6     | 240  | U    | 2.4  |
| 36  | 5     | 3153 | U    | 2.4  |
| 40  | L3    | 200  | GLU  | 2.4  |
| 56  | N0    | 21   | GLU  | 2.4  |
| 12  | c0    | 64   | TYR  | 2.4  |
| 19  | C7    | 14   | LYS  | 2.4  |
| 42  | L5    | 294  | ALA  | 2.4  |
| 44  | L7    | 27   | ALA  | 2.4  |
| 55  | M9    | 133  | LYS  | 2.4  |
| 60  | n4    | 116  | LYS  | 2.4  |
| 60  | n4    | 118  | ALA  | 2.4  |
| 63  | N7    | 2    | ALA  | 2.4  |
| 70  | o4    | 33   | GLN  | 2.4  |
| 16  | C4    | 89   | THR  | 2.4  |
| 33  | E1    | 86   | THR  | 2.4  |
| 7   | s5    | 224  | ASN  | 2.4  |
| 23  | D1    | 75   | ASN  | 2.4  |
| 30  | d8    | 9    | LEU  | 2.4  |
| 1   | 2     | 713  | A    | 2.4  |
| 1   | 6     | 1228 | G    | 2.4  |
| 2   | s0    | 190  | ASP  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | d0    | 20   | ILE  | 2.4  |
| 27  | D5    | 50   | ILE  | 2.4  |
| 82  | p0    | 72   | ASP  | 2.4  |
| 2   | S0    | 50   | VAL  | 2.4  |
| 8   | S6    | 165  | GLY  | 2.4  |
| 9   | S7    | 90   | VAL  | 2.4  |
| 14  | c2    | 63   | VAL  | 2.4  |
| 52  | m6    | 69   | GLY  | 2.4  |
| 42  | l5    | 269  | SER  | 2.4  |
| 45  | L8    | 57   | ARG  | 2.4  |
| 1   | 2     | 822  | U    | 2.4  |
| 1   | 6     | 1710 | U    | 2.4  |
| 11  | S9    | 138  | LYS  | 2.4  |
| 37  | 7     | 121  | U    | 2.4  |
| 50  | m4    | 92   | GLU  | 2.4  |
| 61  | N5    | 22   | LYS  | 2.4  |
| 35  | sM    | 136  | ALA  | 2.4  |
| 19  | C7    | 84   | TYR  | 2.4  |
| 42  | L5    | 297  | GLN  | 2.4  |
| 45  | L8    | 123  | GLN  | 2.4  |
| 12  | C0    | 90   | THR  | 2.4  |
| 18  | c6    | 115  | THR  | 2.4  |
| 58  | n2    | 14   | THR  | 2.4  |
| 20  | C8    | 55   | HIS  | 2.4  |
| 9   | s7    | 16   | LEU  | 2.4  |
| 17  | C5    | 65   | LEU  | 2.4  |
| 35  | SM    | 151  | LEU  | 2.4  |
| 32  | E0    | 51   | ASN  | 2.4  |
| 27  | d5    | 78   | ILE  | 2.4  |
| 30  | d8    | 40   | ILE  | 2.4  |
| 29  | d7    | 37   | CYS  | 2.4  |
| 36  | 1     | 2094 | C    | 2.4  |
| 45  | l8    | 25   | PRO  | 2.4  |
| 2   | S0    | 43   | ASP  | 2.4  |
| 3   | S1    | 91   | VAL  | 2.4  |
| 8   | S6    | 153  | VAL  | 2.4  |
| 9   | S7    | 145  | GLY  | 2.4  |
| 30  | d8    | 7    | VAL  | 2.4  |
| 33  | e1    | 112  | GLY  | 2.4  |
| 38  | 4     | 79   | A    | 2.4  |
| 6   | S4    | 187  | ARG  | 2.4  |
| 7   | S5    | 222  | LYS  | 2.4  |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 50         | m4           | 137        | LYS         | 2.4         |
| 1          | 6            | 1697       | G           | 2.4         |
| 14         | C2           | 109        | GLU         | 2.4         |
| 16         | C4           | 11         | SER         | 2.4         |
| 17         | c5           | 12         | PHE         | 2.4         |
| 18         | c6           | 46         | PHE         | 2.4         |
| 47         | m0           | 217        | PHE         | 2.4         |
| 52         | m6           | 187        | GLU         | 2.4         |
| 3          | S1           | 147        | ALA         | 2.4         |
| 33         | E1           | 110        | ALA         | 2.4         |
| 45         | L8           | 115        | ALA         | 2.4         |
| 45         | l8           | 113        | ALA         | 2.4         |
| 1          | 2            | 912        | U           | 2.4         |
| 1          | 2            | 1657       | U           | 2.4         |
| 16         | c4           | 58         | TYR         | 2.4         |
| 22         | D0           | 67         | THR         | 2.4         |
| 12         | C0           | 85         | HIS         | 2.4         |
| 5          | S3           | 142        | LEU         | 2.4         |
| 14         | C2           | 62         | LEU         | 2.4         |
| 20         | C8           | 32         | LEU         | 2.4         |
| 28         | D6           | 53         | LEU         | 2.4         |
| 66         | o0           | 14         | LEU         | 2.4         |
| 14         | c2           | 24         | ILE         | 2.4         |
| 35         | SM           | 25         | ILE         | 2.4         |
| 66         | o0           | 42         | ILE         | 2.4         |
| 35         | SM           | 86         | ASN         | 2.4         |
| 3          | S1           | 68         | VAL         | 2.4         |
| 8          | S6           | 114        | VAL         | 2.4         |
| 34         | sR           | 104        | VAL         | 2.4         |
| 58         | N2           | 27         | VAL         | 2.4         |
| 5          | S3           | 54         | ARG         | 2.4         |
| 27         | D5           | 48         | ASP         | 2.4         |
| 41         | l4           | 288        | ARG         | 2.4         |
| 45         | L8           | 156        | ASP         | 2.4         |
| 82         | p0           | 48         | ARG         | 2.4         |
| 1          | 2            | 136        | C           | 2.4         |
| 36         | 5            | 1761       | C           | 2.4         |
| 1          | 2            | 217        | A           | 2.4         |
| 16         | C4           | 27         | PHE         | 2.4         |
| 36         | 1            | 2445       | A           | 2.4         |
| 55         | M9           | 179        | GLU         | 2.4         |
| 5          | s3           | 219        | ALA         | 2.4         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | D0    | 105  | GLN  | 2.4  |
| 27  | D5    | 93   | SER  | 2.4  |
| 42  | l5    | 296  | GLN  | 2.4  |
| 47  | m0    | 113  | GLN  | 2.4  |
| 56  | n0    | 138  | GLN  | 2.4  |
| 66  | o0    | 12   | GLN  | 2.4  |
| 72  | O6    | 97   | SER  | 2.4  |
| 1   | 2     | 820  | U    | 2.4  |
| 1   | 2     | 1685 | G    | 2.4  |
| 1   | 6     | 1059 | U    | 2.4  |
| 36  | 1     | 547  | G    | 2.4  |
| 36  | 1     | 1547 | G    | 2.4  |
| 36  | 5     | 251  | G    | 2.4  |
| 36  | 5     | 441  | U    | 2.4  |
| 36  | 5     | 2095 | G    | 2.4  |
| 63  | n7    | 86   | THR  | 2.4  |
| 20  | c8    | 18   | LEU  | 2.4  |
| 3   | S1    | 140  | ILE  | 2.4  |
| 2   | S0    | 4    | PRO  | 2.4  |
| 2   | S0    | 127  | ARG  | 2.3  |
| 3   | S1    | 33   | LYS  | 2.3  |
| 3   | S1    | 94   | LYS  | 2.3  |
| 8   | S6    | 162  | VAL  | 2.3  |
| 23  | D1    | 22   | ARG  | 2.3  |
| 52  | m6    | 3    | VAL  | 2.3  |
| 79  | q3    | 7    | LYS  | 2.3  |
| 34  | sR    | 280  | GLY  | 2.3  |
| 14  | C2    | 128  | ALA  | 2.3  |
| 22  | D0    | 45   | ALA  | 2.3  |
| 55  | M9    | 168  | ALA  | 2.3  |
| 60  | n4    | 125  | ALA  | 2.3  |
| 1   | 2     | 708  | C    | 2.3  |
| 36  | 1     | 1232 | C    | 2.3  |
| 59  | N3    | 7    | GLN  | 2.3  |
| 3   | S1    | 229  | MET  | 2.3  |
| 34  | sR    | 282  | SER  | 2.3  |
| 36  | 5     | 2208 | A    | 2.3  |
| 41  | L4    | 2    | SER  | 2.3  |
| 41  | l4    | 232  | SER  | 2.3  |
| 52  | m6    | 180  | SER  | 2.3  |
| 3   | s1    | 110  | LEU  | 2.3  |
| 16  | C4    | 38   | THR  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | c7    | 117  | LEU  | 2.3  |
| 20  | C8    | 66   | LEU  | 2.3  |
| 35  | SM    | 20   | LEU  | 2.3  |
| 1   | 2     | 502  | U    | 2.3  |
| 1   | 2     | 1059 | U    | 2.3  |
| 1   | 6     | 1058 | U    | 2.3  |
| 36  | 1     | 3079 | U    | 2.3  |
| 36  | 5     | 2097 | U    | 2.3  |
| 31  | d9    | 38   | ILE  | 2.3  |
| 13  | c1    | 29   | LYS  | 2.3  |
| 21  | C9    | 2    | PRO  | 2.3  |
| 22  | D0    | 96   | PRO  | 2.3  |
| 82  | p0    | 23   | LYS  | 2.3  |
| 3   | S1    | 192  | VAL  | 2.3  |
| 8   | S6    | 157  | VAL  | 2.3  |
| 9   | s7    | 109  | VAL  | 2.3  |
| 21  | C9    | 6    | VAL  | 2.3  |
| 28  | d6    | 45   | VAL  | 2.3  |
| 31  | D9    | 6    | VAL  | 2.3  |
| 33  | e1    | 114  | VAL  | 2.3  |
| 36  | 5     | 3288 | G    | 2.3  |
| 58  | n2    | 54   | VAL  | 2.3  |
| 12  | C0    | 19   | GLY  | 2.3  |
| 16  | C4    | 87   | GLY  | 2.3  |
| 8   | s6    | 152  | ASP  | 2.3  |
| 11  | S9    | 106  | GLU  | 2.3  |
| 26  | D4    | 4    | ALA  | 2.3  |
| 27  | D5    | 104  | ALA  | 2.3  |
| 34  | SR    | 78   | ALA  | 2.3  |
| 41  | L4    | 63   | GLU  | 2.3  |
| 42  | L5    | 263  | GLU  | 2.3  |
| 53  | M7    | 2    | ALA  | 2.3  |
| 56  | n0    | 21   | GLU  | 2.3  |
| 70  | o4    | 111  | ALA  | 2.3  |
| 3   | S1    | 97   | LEU  | 2.3  |
| 7   | S5    | 25   | LEU  | 2.3  |
| 11  | S9    | 87   | SER  | 2.3  |
| 12  | c0    | 82   | LEU  | 2.3  |
| 14  | C2    | 41   | LEU  | 2.3  |
| 33  | e1    | 117  | LEU  | 2.3  |
| 41  | L4    | 64   | SER  | 2.3  |
| 45  | L8    | 255  | SER  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 6     | 1703 | C    | 2.3  |
| 2   | S0    | 98   | ILE  | 2.3  |
| 3   | s1    | 126  | THR  | 2.3  |
| 19  | C7    | 69   | ILE  | 2.3  |
| 33  | e1    | 91   | ILE  | 2.3  |
| 36  | 5     | 438  | A    | 2.3  |
| 36  | 5     | 2100 | A    | 2.3  |
| 82  | p0    | 4    | ILE  | 2.3  |
| 14  | c2    | 85   | LYS  | 2.3  |
| 18  | c6    | 23   | LYS  | 2.3  |
| 27  | D5    | 94   | LYS  | 2.3  |
| 49  | M3    | 131  | LYS  | 2.3  |
| 1   | 6     | 73   | U    | 2.3  |
| 36  | 5     | 252  | U    | 2.3  |
| 36  | 5     | 3156 | U    | 2.3  |
| 33  | E1    | 88   | PRO  | 2.3  |
| 19  | C7    | 110  | VAL  | 2.3  |
| 82  | p0    | 214  | VAL  | 2.3  |
| 3   | S1    | 53   | GLY  | 2.3  |
| 31  | D9    | 8    | PHE  | 2.3  |
| 1   | 2     | 729  | G    | 2.3  |
| 1   | 6     | 722  | G    | 2.3  |
| 2   | S0    | 187  | ALA  | 2.3  |
| 8   | s6    | 122  | GLU  | 2.3  |
| 35  | sM    | 47   | ALA  | 2.3  |
| 67  | O1    | 111  | GLU  | 2.3  |
| 74  | o8    | 34   | ALA  | 2.3  |
| 14  | c2    | 107  | ASP  | 2.3  |
| 33  | E1    | 137  | ASP  | 2.3  |
| 8   | S6    | 68   | LEU  | 2.3  |
| 34  | SR    | 9    | LEU  | 2.3  |
| 49  | M3    | 160  | GLN  | 2.3  |
| 7   | s5    | 40   | ILE  | 2.3  |
| 8   | s6    | 115  | LYS  | 2.3  |
| 9   | s7    | 49   | ILE  | 2.3  |
| 22  | d0    | 101  | LYS  | 2.3  |
| 27  | d5    | 71   | ILE  | 2.3  |
| 28  | d6    | 80   | HIS  | 2.3  |
| 33  | E1    | 143  | LYS  | 2.3  |
| 34  | sR    | 136  | ILE  | 2.3  |
| 50  | M4    | 8    | LYS  | 2.3  |
| 10  | S8    | 120  | THR  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | c1    | 27   | THR  | 2.3  |
| 14  | C2    | 67   | THR  | 2.3  |
| 28  | D6    | 67   | THR  | 2.3  |
| 2   | S0    | 165  | ARG  | 2.3  |
| 21  | c9    | 134  | ARG  | 2.3  |
| 53  | m7    | 126  | ARG  | 2.3  |
| 75  | O9    | 46   | ARG  | 2.3  |
| 82  | p0    | 5    | ARG  | 2.3  |
| 1   | 2     | 139  | C    | 2.3  |
| 1   | 6     | 1000 | C    | 2.3  |
| 14  | c2    | 75   | VAL  | 2.3  |
| 36  | 1     | 1562 | C    | 2.3  |
| 36  | 1     | 1761 | C    | 2.3  |
| 36  | 1     | 2265 | C    | 2.3  |
| 1   | 2     | 1052 | U    | 2.3  |
| 1   | 2     | 1361 | U    | 2.3  |
| 1   | 6     | 74   | U    | 2.3  |
| 1   | 6     | 241  | U    | 2.3  |
| 1   | 6     | 675  | U    | 2.3  |
| 36  | 1     | 2542 | U    | 2.3  |
| 36  | 1     | 3355 | U    | 2.3  |
| 36  | 5     | 1567 | U    | 2.3  |
| 36  | 5     | 1575 | A    | 2.3  |
| 33  | E1    | 129  | GLY  | 2.3  |
| 42  | l5    | 295  | GLY  | 2.3  |
| 78  | Q2    | 101  | GLY  | 2.3  |
| 45  | l8    | 24   | ASN  | 2.3  |
| 4   | S2    | 249  | ALA  | 2.3  |
| 5   | s3    | 118  | ALA  | 2.3  |
| 8   | S6    | 138  | ALA  | 2.3  |
| 14  | C2    | 112  | ALA  | 2.3  |
| 16  | C4    | 40   | ALA  | 2.3  |
| 29  | d7    | 57   | GLU  | 2.3  |
| 41  | l4    | 101  | ALA  | 2.3  |
| 47  | M0    | 102  | MET  | 2.3  |
| 12  | C0    | 93   | GLN  | 2.3  |
| 20  | C8    | 3    | LEU  | 2.3  |
| 21  | C9    | 28   | LEU  | 2.3  |
| 27  | d5    | 43   | ASP  | 2.3  |
| 35  | sM    | 157  | GLN  | 2.3  |
| 9   | S7    | 7    | LYS  | 2.3  |
| 9   | S7    | 157  | LYS  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 55         | m9           | 186        | LYS         | 2.3         |
| 58         | n2           | 70         | LYS         | 2.3         |
| 36         | 5            | 236        | G           | 2.3         |
| 36         | 5            | 547        | G           | 2.3         |
| 42         | l5           | 290        | ILE         | 2.3         |
| 66         | O0           | 100        | ILE         | 2.3         |
| 14         | c2           | 23         | THR         | 2.3         |
| 22         | D0           | 66         | SER         | 2.3         |
| 26         | D4           | 2          | SER         | 2.3         |
| 35         | sM           | 79         | SER         | 2.3         |
| 45         | L8           | 84         | ARG         | 2.3         |
| 45         | L8           | 253        | SER         | 2.3         |
| 55         | m9           | 85         | ARG         | 2.3         |
| 2          | S0           | 138        | TYR         | 2.3         |
| 9          | s7           | 51         | VAL         | 2.3         |
| 14         | c2           | 30         | VAL         | 2.3         |
| 19         | C7           | 124        | VAL         | 2.3         |
| 30         | D8           | 25         | VAL         | 2.3         |
| 35         | SM           | 166        | VAL         | 2.3         |
| 25         | D3           | 2          | GLY         | 2.3         |
| 52         | M6           | 69         | GLY         | 2.3         |
| 59         | N3           | 5          | GLY         | 2.3         |
| 82         | p0           | 194        | GLY         | 2.3         |
| 1          | 6            | 232        | U           | 2.3         |
| 36         | 1            | 2541       | U           | 2.3         |
| 36         | 1            | 2571       | U           | 2.3         |
| 36         | 5            | 240        | U           | 2.3         |
| 1          | 2            | 1634       | C           | 2.2         |
| 1          | 6            | 1700       | C           | 2.2         |
| 9          | S7           | 61         | PHE         | 2.2         |
| 36         | 1            | 2093       | A           | 2.2         |
| 36         | 1            | 2101       | C           | 2.2         |
| 36         | 5            | 1556       | C           | 2.2         |
| 36         | 5            | 2098       | C           | 2.2         |
| 15         | C3           | 148        | ALA         | 2.2         |
| 26         | d4           | 130        | ALA         | 2.2         |
| 28         | D6           | 35         | ALA         | 2.2         |
| 28         | D6           | 48         | ALA         | 2.2         |
| 35         | sM           | 120        | GLU         | 2.2         |
| 52         | M6           | 40         | GLU         | 2.2         |
| 58         | n2           | 44         | GLU         | 2.2         |
| 60         | n4           | 111        | ALA         | 2.2         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 70  | o4    | 2    | ALA  | 2.2  |
| 82  | p0    | 44   | GLU  | 2.2  |
| 5   | S3    | 72   | LEU  | 2.2  |
| 27  | D5    | 75   | LEU  | 2.2  |
| 8   | S6    | 214  | LYS  | 2.2  |
| 9   | s7    | 11   | GLN  | 2.2  |
| 60  | N4    | 91   | LYS  | 2.2  |
| 2   | s0    | 129  | ASP  | 2.2  |
| 26  | D4    | 135  | ASP  | 2.2  |
| 18  | C6    | 66   | ARG  | 2.2  |
| 26  | d4    | 132  | ARG  | 2.2  |
| 60  | n4    | 43   | ARG  | 2.2  |
| 9   | S7    | 14   | THR  | 2.2  |
| 20  | c8    | 93   | THR  | 2.2  |
| 5   | s3    | 41   | VAL  | 2.2  |
| 6   | s4    | 183  | VAL  | 2.2  |
| 14  | c2    | 141  | SER  | 2.2  |
| 16  | C4    | 96   | PRO  | 2.2  |
| 19  | C7    | 121  | VAL  | 2.2  |
| 22  | D0    | 51   | VAL  | 2.2  |
| 22  | d0    | 116  | VAL  | 2.2  |
| 1   | 2     | 234  | G    | 2.2  |
| 1   | 6     | 834  | G    | 2.2  |
| 36  | 1     | 1573 | G    | 2.2  |
| 8   | s6    | 165  | GLY  | 2.2  |
| 47  | m0    | 114  | GLY  | 2.2  |
| 71  | O5    | 3    | GLY  | 2.2  |
| 2   | S0    | 198  | MET  | 2.2  |
| 1   | 2     | 504  | U    | 2.2  |
| 1   | 2     | 507  | U    | 2.2  |
| 1   | 2     | 705  | U    | 2.2  |
| 1   | 2     | 1491 | U    | 2.2  |
| 36  | 1     | 2538 | U    | 2.2  |
| 36  | 5     | 1950 | U    | 2.2  |
| 5   | s3    | 218  | LEU  | 2.2  |
| 8   | s6    | 35   | GLU  | 2.2  |
| 9   | S7    | 15   | GLU  | 2.2  |
| 16  | C4    | 100  | ALA  | 2.2  |
| 27  | D5    | 39   | ALA  | 2.2  |
| 34  | SR    | 36   | ALA  | 2.2  |
| 45  | l8    | 211  | LEU  | 2.2  |
| 49  | m3    | 134  | GLU  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 52         | M6           | 166        | GLU         | 2.2         |
| 63         | N7           | 59         | ALA         | 2.2         |
| 16         | c4           | 92         | LYS         | 2.2         |
| 34         | sR           | 4          | ASN         | 2.2         |
| 34         | sR           | 252        | LEU         | 2.2         |
| 36         | 5            | 235        | A           | 2.2         |
| 54         | m8           | 145        | ASN         | 2.2         |
| 20         | C8           | 35         | ILE         | 2.2         |
| 31         | D9           | 50         | ILE         | 2.2         |
| 3          | s1           | 232        | HIS         | 2.2         |
| 7          | s5           | 161        | ASP         | 2.2         |
| 55         | M9           | 85         | ARG         | 2.2         |
| 55         | M9           | 181        | ARG         | 2.2         |
| 2          | S0           | 31         | VAL         | 2.2         |
| 9          | s7           | 63         | PRO         | 2.2         |
| 11         | S9           | 2          | PRO         | 2.2         |
| 12         | c0           | 22         | VAL         | 2.2         |
| 16         | C4           | 16         | VAL         | 2.2         |
| 18         | c6           | 37         | THR         | 2.2         |
| 19         | c7           | 55         | THR         | 2.2         |
| 34         | SR           | 12         | THR         | 2.2         |
| 82         | p0           | 3          | GLY         | 2.2         |
| 47         | m0           | 102        | MET         | 2.2         |
| 42         | L5           | 260        | PHE         | 2.2         |
| 4          | S2           | 247        | ALA         | 2.2         |
| 6          | s4           | 133        | LYS         | 2.2         |
| 11         | s9           | 116        | LEU         | 2.2         |
| 41         | l4           | 305        | ALA         | 2.2         |
| 46         | l9           | 189        | GLU         | 2.2         |
| 53         | M7           | 183        | ALA         | 2.2         |
| 55         | M9           | 186        | LYS         | 2.2         |
| 66         | O0           | 105        | ALA         | 2.2         |
| 67         | o1           | 85         | ALA         | 2.2         |
| 74         | o8           | 26         | LYS         | 2.2         |
| 21         | c9           | 144        | GLU         | 2.2         |
| 36         | 1            | 1953       | G           | 2.2         |
| 36         | 1            | 2503       | G           | 2.2         |
| 78         | Q2           | 104        | LEU         | 2.2         |
| 1          | 6            | 1362       | U           | 2.2         |
| 36         | 1            | 1356       | U           | 2.2         |
| 36         | 5            | 3277       | U           | 2.2         |
| 38         | 8            | 158        | U           | 2.2         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | C3    | 151  | ASN  | 2.2  |
| 18  | C6    | 62   | ASN  | 2.2  |
| 23  | D1    | 21   | ASN  | 2.2  |
| 2   | S0    | 205  | ARG  | 2.2  |
| 8   | S6    | 18   | ILE  | 2.2  |
| 9   | S7    | 74   | GLN  | 2.2  |
| 9   | s7    | 108  | GLN  | 2.2  |
| 22  | D0    | 15   | GLN  | 2.2  |
| 22  | d0    | 91   | ILE  | 2.2  |
| 1   | 6     | 1756 | A    | 2.2  |
| 36  | 1     | 1583 | A    | 2.2  |
| 1   | 6     | 717  | C    | 2.2  |
| 36  | 1     | 1563 | C    | 2.2  |
| 36  | 1     | 2098 | C    | 2.2  |
| 36  | 5     | 2539 | C    | 2.2  |
| 36  | 5     | 3278 | C    | 2.2  |
| 12  | c0    | 87   | VAL  | 2.2  |
| 33  | E1    | 147  | VAL  | 2.2  |
| 69  | o3    | 90   | PRO  | 2.2  |
| 9   | s7    | 14   | THR  | 2.2  |
| 31  | D9    | 7    | TRP  | 2.2  |
| 6   | S4    | 25   | GLY  | 2.2  |
| 17  | C5    | 28   | MET  | 2.2  |
| 9   | s7    | 30   | SER  | 2.2  |
| 14  | c2    | 55   | GLY  | 2.2  |
| 35  | sM    | 56   | GLY  | 2.2  |
| 41  | l4    | 68   | GLY  | 2.2  |
| 41  | l4    | 85   | SER  | 2.2  |
| 58  | n2    | 108  | TYR  | 2.2  |
| 5   | S3    | 212  | LYS  | 2.2  |
| 27  | d5    | 97   | LYS  | 2.2  |
| 39  | l2    | 16   | PHE  | 2.2  |
| 67  | o1    | 86   | LYS  | 2.2  |
| 23  | D1    | 55   | LEU  | 2.2  |
| 26  | D4    | 125  | LEU  | 2.2  |
| 50  | m4    | 135  | LEU  | 2.2  |
| 55  | m9    | 164  | LEU  | 2.2  |
| 4   | S2    | 120  | GLU  | 2.2  |
| 9   | s7    | 36   | ALA  | 2.2  |
| 9   | s7    | 59   | ALA  | 2.2  |
| 17  | c5    | 131  | ALA  | 2.2  |
| 43  | l6    | 129  | GLU  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 260  | U    | 2.2  |
| 1   | 2     | 681  | U    | 2.2  |
| 10  | s8    | 8    | ARG  | 2.2  |
| 76  | Q0    | 77   | ILE  | 2.2  |
| 82  | p0    | 63   | ILE  | 2.2  |
| 22  | D0    | 98   | GLN  | 2.2  |
| 36  | 1     | 1094 | U    | 2.2  |
| 42  | L5    | 296  | GLN  | 2.2  |
| 1   | 6     | 235  | G    | 2.2  |
| 18  | c6    | 21   | HIS  | 2.2  |
| 1   | 6     | 1702 | A    | 2.2  |
| 14  | c2    | 121  | VAL  | 2.2  |
| 15  | C3    | 108  | ASP  | 2.2  |
| 34  | SR    | 165  | ASP  | 2.2  |
| 36  | 1     | 2443 | A    | 2.2  |
| 67  | O1    | 112  | ASP  | 2.2  |
| 72  | o6    | 3    | VAL  | 2.2  |
| 1   | 2     | 704  | C    | 2.2  |
| 14  | c2    | 137  | MET  | 2.2  |
| 30  | d8    | 5    | THR  | 2.2  |
| 78  | Q2    | 78   | LYS  | 2.2  |
| 58  | N2    | 83   | TYR  | 2.2  |
| 6   | S4    | 123  | LEU  | 2.2  |
| 16  | C4    | 55   | SER  | 2.2  |
| 16  | C4    | 137  | LEU  | 2.2  |
| 18  | c6    | 52   | LEU  | 2.2  |
| 30  | D8    | 54   | LEU  | 2.2  |
| 82  | p0    | 76   | LEU  | 2.2  |
| 9   | S7    | 33   | GLU  | 2.2  |
| 18  | c6    | 24   | ALA  | 2.2  |
| 26  | D4    | 101  | GLU  | 2.2  |
| 26  | d4    | 98   | GLU  | 2.2  |
| 35  | SM    | 135  | ALA  | 2.2  |
| 35  | sM    | 137  | GLU  | 2.2  |
| 2   | s0    | 41   | ARG  | 2.1  |
| 2   | s0    | 185  | ARG  | 2.1  |
| 5   | S3    | 209  | ILE  | 2.1  |
| 18  | C6    | 68   | ARG  | 2.1  |
| 22  | d0    | 103  | ILE  | 2.1  |
| 48  | M1    | 60   | ARG  | 2.1  |
| 3   | S1    | 92   | GLN  | 2.1  |
| 22  | d0    | 12   | GLN  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | m9    | 150  | GLN  | 2.1  |
| 1   | 2     | 779  | U    | 2.1  |
| 8   | S6    | 80   | ASN  | 2.1  |
| 36  | 1     | 1820 | U    | 2.1  |
| 36  | 5     | 1572 | U    | 2.1  |
| 2   | S0    | 35   | PRO  | 2.1  |
| 3   | S1    | 21   | VAL  | 2.1  |
| 4   | S2    | 85   | PRO  | 2.1  |
| 8   | s6    | 153  | VAL  | 2.1  |
| 9   | S7    | 64   | VAL  | 2.1  |
| 82  | p0    | 99   | VAL  | 2.1  |
| 11  | S9    | 63   | ASP  | 2.1  |
| 1   | 2     | 723  | G    | 2.1  |
| 8   | S6    | 194  | LYS  | 2.1  |
| 8   | S6    | 223  | LYS  | 2.1  |
| 14  | C2    | 50   | LYS  | 2.1  |
| 18  | c6    | 17   | THR  | 2.1  |
| 20  | C8    | 80   | LYS  | 2.1  |
| 25  | D3    | 114  | LYS  | 2.1  |
| 26  | D4    | 127  | LYS  | 2.1  |
| 34  | sR    | 125  | GLY  | 2.1  |
| 36  | 1     | 1093 | A    | 2.1  |
| 36  | 1     | 1246 | G    | 2.1  |
| 36  | 1     | 1566 | A    | 2.1  |
| 36  | 1     | 2502 | A    | 2.1  |
| 36  | 5     | 170  | G    | 2.1  |
| 36  | 5     | 1577 | G    | 2.1  |
| 45  | L8    | 120  | LYS  | 2.1  |
| 45  | L8    | 251  | LYS  | 2.1  |
| 60  | n4    | 124  | LYS  | 2.1  |
| 1   | 6     | 684  | A    | 2.1  |
| 3   | s1    | 178  | GLY  | 2.1  |
| 36  | 5     | 2093 | A    | 2.1  |
| 36  | 5     | 3347 | A    | 2.1  |
| 41  | L4    | 79   | GLY  | 2.1  |
| 34  | sR    | 294  | TRP  | 2.1  |
| 1   | 6     | 1537 | C    | 2.1  |
| 4   | S2    | 154  | LEU  | 2.1  |
| 14  | C2    | 28   | LEU  | 2.1  |
| 28  | D6    | 62   | TYR  | 2.1  |
| 36  | 5     | 3166 | C    | 2.1  |
| 78  | q2    | 106  | PHE  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | S5    | 74   | ALA  | 2.1  |
| 12  | c0    | 89   | ALA  | 2.1  |
| 20  | c8    | 2    | SER  | 2.1  |
| 23  | D1    | 18   | SER  | 2.1  |
| 34  | SR    | 95   | ALA  | 2.1  |
| 34  | sR    | 35   | SER  | 2.1  |
| 42  | L5    | 291  | ALA  | 2.1  |
| 44  | l7    | 23   | ALA  | 2.1  |
| 45  | l8    | 253  | SER  | 2.1  |
| 40  | L3    | 94   | GLU  | 2.1  |
| 60  | n4    | 114  | GLU  | 2.1  |
| 67  | o1    | 111  | GLU  | 2.1  |
| 33  | E1    | 91   | ILE  | 2.1  |
| 60  | N4    | 82   | ILE  | 2.1  |
| 8   | s6    | 80   | ASN  | 2.1  |
| 28  | D6    | 11   | ASN  | 2.1  |
| 82  | p0    | 103  | ASN  | 2.1  |
| 2   | s0    | 42   | PRO  | 2.1  |
| 27  | d5    | 40   | VAL  | 2.1  |
| 36  | 5     | 492  | U    | 2.1  |
| 45  | l8    | 246  | MET  | 2.1  |
| 8   | s6    | 167  | LYS  | 2.1  |
| 19  | c7    | 116  | LYS  | 2.1  |
| 26  | D4    | 117  | LYS  | 2.1  |
| 5   | S3    | 204  | ASP  | 2.1  |
| 14  | c2    | 102  | GLY  | 2.1  |
| 34  | sR    | 28   | GLY  | 2.1  |
| 43  | l6    | 67   | GLY  | 2.1  |
| 49  | m3    | 152  | THR  | 2.1  |
| 19  | c7    | 119  | LEU  | 2.1  |
| 34  | SR    | 61   | PHE  | 2.1  |
| 58  | N2    | 28   | PHE  | 2.1  |
| 72  | o6    | 11   | LEU  | 2.1  |
| 1   | 2     | 1346 | A    | 2.1  |
| 3   | S1    | 26   | ARG  | 2.1  |
| 11  | S9    | 183  | ALA  | 2.1  |
| 18  | C6    | 142  | TYR  | 2.1  |
| 20  | C8    | 83   | ALA  | 2.1  |
| 36  | 1     | 2096 | A    | 2.1  |
| 36  | 5     | 1566 | A    | 2.1  |
| 63  | n7    | 2    | ALA  | 2.1  |
| 66  | o0    | 105  | ALA  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 540  | G    | 2.1  |
| 1   | 6     | 652  | G    | 2.1  |
| 2   | S0    | 111  | ILE  | 2.1  |
| 11  | S9    | 186  | GLU  | 2.1  |
| 36  | 1     | 439  | C    | 2.1  |
| 36  | 1     | 765  | C    | 2.1  |
| 7   | s5    | 158  | GLN  | 2.1  |
| 78  | Q2    | 105  | GLN  | 2.1  |
| 82  | p0    | 195  | GLN  | 2.1  |
| 20  | C8    | 78   | HIS  | 2.1  |
| 3   | S1    | 43   | VAL  | 2.1  |
| 7   | S5    | 59   | VAL  | 2.1  |
| 7   | s5    | 41   | LYS  | 2.1  |
| 8   | S6    | 129  | VAL  | 2.1  |
| 8   | S6    | 179  | VAL  | 2.1  |
| 11  | S9    | 148  | VAL  | 2.1  |
| 14  | c2    | 37   | VAL  | 2.1  |
| 15  | c3    | 150  | VAL  | 2.1  |
| 33  | e1    | 82   | LYS  | 2.1  |
| 48  | M1    | 8    | PRO  | 2.1  |
| 48  | m1    | 8    | PRO  | 2.1  |
| 1   | 6     | 666  | U    | 2.1  |
| 1   | 6     | 792  | U    | 2.1  |
| 36  | 1     | 1348 | U    | 2.1  |
| 36  | 5     | 3195 | U    | 2.1  |
| 4   | S2    | 145  | GLY  | 2.1  |
| 16  | C4    | 33   | LEU  | 2.1  |
| 29  | D7    | 33   | LEU  | 2.1  |
| 10  | s8    | 109  | PHE  | 2.1  |
| 14  | c2    | 130  | THR  | 2.1  |
| 17  | C5    | 50   | THR  | 2.1  |
| 29  | d7    | 61   | THR  | 2.1  |
| 34  | SR    | 99   | THR  | 2.1  |
| 64  | N8    | 98   | THR  | 2.1  |
| 15  | c3    | 104  | ARG  | 2.1  |
| 19  | C7    | 80   | ARG  | 2.1  |
| 55  | M9    | 5    | ARG  | 2.1  |
| 2   | S0    | 99   | ALA  | 2.1  |
| 16  | C4    | 101  | ALA  | 2.1  |
| 18  | c6    | 18   | ALA  | 2.1  |
| 29  | d7    | 62   | ILE  | 2.1  |
| 35  | sM    | 138  | ALA  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | L4    | 72   | ALA  | 2.1  |
| 70  | o4    | 75   | ALA  | 2.1  |
| 15  | c3    | 83   | GLU  | 2.1  |
| 19  | C7    | 75   | GLU  | 2.1  |
| 35  | sM    | 139  | GLU  | 2.1  |
| 82  | p0    | 22   | TYR  | 2.1  |
| 82  | p0    | 191  | TYR  | 2.1  |
| 1   | 2     | 1492 | A    | 2.1  |
| 25  | d3    | 145  | SER  | 2.1  |
| 36  | 1     | 980  | A    | 2.1  |
| 4   | s2    | 89   | GLN  | 2.1  |
| 57  | N1    | 103  | GLN  | 2.1  |
| 1   | 2     | 559  | C    | 2.1  |
| 1   | 2     | 720  | G    | 2.1  |
| 1   | 2     | 1718 | G    | 2.1  |
| 1   | 6     | 234  | G    | 2.1  |
| 1   | 6     | 913  | G    | 2.1  |
| 7   | S5    | 54   | LYS  | 2.1  |
| 10  | s8    | 137  | LYS  | 2.1  |
| 14  | c2    | 114  | LYS  | 2.1  |
| 20  | c8    | 55   | HIS  | 2.1  |
| 28  | D6    | 84   | VAL  | 2.1  |
| 34  | SR    | 46   | LYS  | 2.1  |
| 35  | SM    | 105  | LYS  | 2.1  |
| 36  | 1     | 2533 | G    | 2.1  |
| 36  | 5     | 2444 | C    | 2.1  |
| 19  | C7    | 88   | VAL  | 2.1  |
| 19  | C7    | 99   | VAL  | 2.1  |
| 2   | S0    | 42   | PRO  | 2.1  |
| 9   | s7    | 40   | PRO  | 2.1  |
| 5   | S3    | 59   | LEU  | 2.1  |
| 14  | c2    | 133  | LEU  | 2.1  |
| 1   | 2     | 241  | U    | 2.1  |
| 1   | 2     | 721  | U    | 2.1  |
| 1   | 2     | 821  | U    | 2.1  |
| 25  | D3    | 4    | GLY  | 2.1  |
| 36  | 1     | 3341 | U    | 2.1  |
| 41  | l4    | 78   | GLY  | 2.1  |
| 63  | n7    | 92   | PHE  | 2.1  |
| 4   | S2    | 141  | ARG  | 2.1  |
| 7   | s5    | 21   | THR  | 2.1  |
| 7   | s5    | 38   | THR  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | S7    | 105  | THR  | 2.1  |
| 9   | s7    | 79   | ARG  | 2.1  |
| 26  | D4    | 90   | ARG  | 2.1  |
| 33  | e1    | 86   | THR  | 2.1  |
| 55  | M9    | 148  | ASP  | 2.1  |
| 6   | S4    | 162  | ILE  | 2.1  |
| 7   | S5    | 40   | ILE  | 2.1  |
| 35  | SM    | 138  | ALA  | 2.1  |
| 35  | sM    | 132  | ALA  | 2.1  |
| 18  | c6    | 40   | GLU  | 2.1  |
| 57  | n1    | 104  | GLU  | 2.1  |
| 19  | C7    | 53   | TYR  | 2.1  |
| 40  | L3    | 154  | TYR  | 2.1  |
| 5   | s3    | 148  | LYS  | 2.0  |
| 12  | c0    | 93   | GLN  | 2.0  |
| 13  | c1    | 32   | LYS  | 2.0  |
| 26  | d4    | 123  | LYS  | 2.0  |
| 39  | L2    | 251  | LYS  | 2.0  |
| 39  | l2    | 249  | SER  | 2.0  |
| 42  | L5    | 5    | LYS  | 2.0  |
| 58  | N2    | 10   | LYS  | 2.0  |
| 66  | O0    | 9    | SER  | 2.0  |
| 66  | o0    | 9    | SER  | 2.0  |
| 22  | D0    | 48   | HIS  | 2.0  |
| 22  | d0    | 15   | GLN  | 2.0  |
| 1   | 2     | 579  | A    | 2.0  |
| 1   | 6     | 1346 | A    | 2.0  |
| 2   | s0    | 45   | VAL  | 2.0  |
| 7   | s5    | 168  | VAL  | 2.0  |
| 11  | S9    | 101  | VAL  | 2.0  |
| 14  | C2    | 115  | VAL  | 2.0  |
| 82  | p0    | 27   | VAL  | 2.0  |
| 11  | s9    | 2    | PRO  | 2.0  |
| 22  | D0    | 110  | PRO  | 2.0  |
| 28  | d6    | 97   | PRO  | 2.0  |
| 45  | L8    | 25   | PRO  | 2.0  |
| 74  | o8    | 37   | PRO  | 2.0  |
| 1   | 2     | 736  | C    | 2.0  |
| 14  | C2    | 103  | LEU  | 2.0  |
| 27  | D5    | 65   | LEU  | 2.0  |
| 30  | d8    | 66   | LEU  | 2.0  |
| 36  | 1     | 1578 | C    | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 1     | 2821 | C    | 2.0  |
| 55  | M9    | 164  | LEU  | 2.0  |
| 1   | 6     | 655  | G    | 2.0  |
| 1   | 6     | 1692 | G    | 2.0  |
| 2   | s0    | 44   | GLY  | 2.0  |
| 9   | S7    | 54   | GLY  | 2.0  |
| 9   | s7    | 85   | PHE  | 2.0  |
| 15  | C3    | 104  | ARG  | 2.0  |
| 16  | C4    | 109  | GLY  | 2.0  |
| 29  | d7    | 17   | ARG  | 2.0  |
| 32  | E0    | 52   | GLY  | 2.0  |
| 36  | 1     | 1565 | G    | 2.0  |
| 42  | l5    | 185  | PHE  | 2.0  |
| 45  | L8    | 119  | GLY  | 2.0  |
| 53  | M7    | 167  | ARG  | 2.0  |
| 8   | s6    | 141  | ILE  | 2.0  |
| 14  | C2    | 81   | ASP  | 2.0  |
| 21  | C9    | 35   | ASP  | 2.0  |
| 24  | D2    | 86   | ILE  | 2.0  |
| 36  | 1     | 249  | U    | 2.0  |
| 36  | 1     | 2537 | U    | 2.0  |
| 36  | 5     | 2537 | U    | 2.0  |
| 39  | l2    | 48   | ILE  | 2.0  |
| 6   | s4    | 2    | ALA  | 2.0  |
| 32  | E0    | 2    | ALA  | 2.0  |
| 71  | O5    | 8    | GLU  | 2.0  |
| 10  | S8    | 151  | LYS  | 2.0  |
| 10  | s8    | 117  | TYR  | 2.0  |
| 33  | e1    | 116  | LYS  | 2.0  |
| 34  | SR    | 137  | LYS  | 2.0  |
| 42  | L5    | 279  | LYS  | 2.0  |
| 74  | O8    | 29   | LYS  | 2.0  |
| 15  | c3    | 72   | MET  | 2.0  |
| 9   | S7    | 11   | GLN  | 2.0  |
| 11  | s9    | 148  | VAL  | 2.0  |
| 34  | SR    | 58   | VAL  | 2.0  |
| 39  | l2    | 19   | HIS  | 2.0  |
| 70  | O4    | 5    | VAL  | 2.0  |
| 2   | S0    | 162  | CYS  | 2.0  |
| 19  | C7    | 22   | PRO  | 2.0  |
| 1   | 2     | 76   | A    | 2.0  |
| 1   | 2     | 1081 | A    | 2.0  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 1797 | A    | 2.0  |
| 1   | 6     | 226  | A    | 2.0  |
| 1   | 6     | 673  | A    | 2.0  |
| 2   | s0    | 9    | LEU  | 2.0  |
| 18  | c6    | 44   | LEU  | 2.0  |
| 19  | c7    | 113  | LEU  | 2.0  |
| 23  | D1    | 62   | ARG  | 2.0  |
| 26  | D4    | 132  | ARG  | 2.0  |
| 30  | D8    | 43   | ASN  | 2.0  |
| 43  | L6    | 97   | ASN  | 2.0  |
| 7   | S5    | 48   | PHE  | 2.0  |
| 20  | C8    | 9    | GLY  | 2.0  |
| 28  | D6    | 79   | ILE  | 2.0  |
| 3   | S1    | 98   | THR  | 2.0  |
| 6   | S4    | 217  | THR  | 2.0  |
| 7   | S5    | 125  | THR  | 2.0  |
| 9   | S7    | 36   | ALA  | 2.0  |
| 16  | C4    | 17   | ALA  | 2.0  |
| 34  | SR    | 284  | ALA  | 2.0  |
| 42  | l5    | 275  | THR  | 2.0  |
| 49  | m3    | 151  | ALA  | 2.0  |
| 60  | N4    | 83   | THR  | 2.0  |
| 65  | N9    | 26   | THR  | 2.0  |
| 1   | 2     | 795  | U    | 2.0  |
| 1   | 6     | 558  | U    | 2.0  |
| 35  | sM    | 78   | ASP  | 2.0  |
| 1   | 2     | 677  | G    | 2.0  |
| 11  | S9    | 65   | LYS  | 2.0  |
| 14  | C2    | 105  | LYS  | 2.0  |
| 22  | d0    | 21   | LYS  | 2.0  |
| 36  | 5     | 183  | G    | 2.0  |
| 36  | 5     | 244  | G    | 2.0  |
| 3   | S1    | 133  | TYR  | 2.0  |
| 33  | E1    | 148  | TYR  | 2.0  |
| 7   | s5    | 220  | VAL  | 2.0  |
| 16  | C4    | 42   | VAL  | 2.0  |
| 16  | C4    | 79   | VAL  | 2.0  |
| 22  | d0    | 42   | VAL  | 2.0  |
| 29  | D7    | 2    | VAL  | 2.0  |
| 79  | Q3    | 71   | VAL  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 85  | MG   | 1     | 3809 | 1/1   | -0.57 | 0.52 | 162,162,162,162            | 0     |
| 85  | MG   | 1     | 3405 | 1/1   | 0.30  | 0.51 | 95,95,95,95                | 0     |
| 85  | MG   | 5     | 3803 | 1/1   | 0.31  | 0.24 | 132,132,132,132            | 0     |
| 85  | MG   | 2     | 1960 | 1/1   | 0.32  | 0.50 | 87,87,87,87                | 0     |
| 85  | MG   | 6     | 2015 | 1/1   | 0.34  | 0.33 | 104,104,104,104            | 0     |
| 85  | MG   | 2     | 1954 | 1/1   | 0.34  | 0.56 | 87,87,87,87                | 0     |
| 85  | MG   | 5     | 3770 | 1/1   | 0.40  | 0.36 | 70,70,70,70                | 0     |
| 85  | MG   | 2     | 2003 | 1/1   | 0.44  | 0.39 | 96,96,96,96                | 0     |
| 85  | MG   | 2     | 1991 | 1/1   | 0.44  | 0.48 | 102,102,102,102            | 0     |
| 85  | MG   | 2     | 1968 | 1/1   | 0.45  | 0.54 | 97,97,97,97                | 0     |
| 85  | MG   | 5     | 3794 | 1/1   | 0.50  | 0.30 | 64,64,64,64                | 0     |
| 85  | MG   | 1     | 3652 | 1/1   | 0.51  | 0.48 | 84,84,84,84                | 0     |
| 85  | MG   | 2     | 1955 | 1/1   | 0.51  | 0.31 | 79,79,79,79                | 0     |
| 85  | MG   | 4     | 220  | 1/1   | 0.52  | 0.40 | 77,77,77,77                | 0     |
| 85  | MG   | 1     | 3863 | 1/1   | 0.53  | 0.13 | 118,118,118,118            | 0     |
| 85  | MG   | 1     | 3593 | 1/1   | 0.54  | 0.32 | 59,59,59,59                | 0     |
| 85  | MG   | 6     | 1924 | 1/1   | 0.55  | 0.58 | 87,87,87,87                | 0     |
| 85  | MG   | 5     | 3896 | 1/1   | 0.56  | 0.27 | 82,82,82,82                | 0     |
| 85  | MG   | 5     | 3466 | 1/1   | 0.57  | 0.53 | 88,88,88,88                | 0     |
| 85  | MG   | 5     | 3773 | 1/1   | 0.57  | 0.33 | 83,83,83,83                | 0     |
| 85  | MG   | 5     | 3781 | 1/1   | 0.57  | 0.27 | 64,64,64,64                | 0     |
| 85  | MG   | 5     | 3707 | 1/1   | 0.58  | 0.44 | 75,75,75,75                | 0     |
| 85  | MG   | 5     | 3846 | 1/1   | 0.59  | 0.33 | 50,50,50,50                | 0     |
| 85  | MG   | 3     | 212  | 1/1   | 0.59  | 0.17 | 63,63,63,63                | 0     |
| 85  | MG   | 6     | 2040 | 1/1   | 0.60  | 0.52 | 82,82,82,82                | 0     |
| 85  | MG   | 2     | 2023 | 1/1   | 0.61  | 0.38 | 101,101,101,101            | 0     |
| 85  | MG   | N5    | 201  | 1/1   | 0.61  | 0.26 | 61,61,61,61                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 1909 | 1/1   | 0.62 | 0.38 | 79,79,79,79                 | 0     |
| 85  | MG   | 5     | 3661 | 1/1   | 0.63 | 0.49 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3881 | 1/1   | 0.63 | 0.51 | 81,81,81,81                 | 0     |
| 85  | MG   | 5     | 3791 | 1/1   | 0.63 | 0.27 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3649 | 1/1   | 0.65 | 0.38 | 59,59,59,59                 | 0     |
| 85  | MG   | 2     | 1975 | 1/1   | 0.65 | 0.50 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3756 | 1/1   | 0.65 | 0.31 | 91,91,91,91                 | 0     |
| 85  | MG   | 2     | 2010 | 1/1   | 0.66 | 0.40 | 62,62,62,62                 | 0     |
| 85  | MG   | 1     | 3833 | 1/1   | 0.67 | 0.12 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3820 | 1/1   | 0.67 | 0.47 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 4236 | 7/7   | 0.67 | 0.25 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3418 | 1/1   | 0.68 | 0.24 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3419 | 1/1   | 0.68 | 0.28 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 3643 | 1/1   | 0.68 | 0.17 | 39,39,39,39                 | 0     |
| 85  | MG   | 2     | 1969 | 1/1   | 0.68 | 0.29 | 79,79,79,79                 | 0     |
| 85  | MG   | 6     | 2021 | 1/1   | 0.69 | 0.31 | 93,93,93,93                 | 0     |
| 85  | MG   | 2     | 1967 | 1/1   | 0.69 | 0.34 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3861 | 1/1   | 0.69 | 0.26 | 65,65,65,65                 | 0     |
| 85  | MG   | 2     | 1915 | 1/1   | 0.69 | 0.41 | 53,53,53,53                 | 0     |
| 85  | MG   | 3     | 209  | 1/1   | 0.69 | 0.34 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3704 | 1/1   | 0.69 | 0.32 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3443 | 1/1   | 0.70 | 0.29 | 65,65,65,65                 | 0     |
| 85  | MG   | 2     | 1972 | 1/1   | 0.70 | 0.35 | 66,66,66,66                 | 0     |
| 85  | MG   | 7     | 213  | 1/1   | 0.70 | 0.12 | 44,44,44,44                 | 0     |
| 85  | MG   | n8    | 201  | 1/1   | 0.70 | 0.12 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3419 | 1/1   | 0.70 | 0.35 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3717 | 1/1   | 0.71 | 0.32 | 58,58,58,58                 | 0     |
| 85  | MG   | 5     | 3727 | 1/1   | 0.71 | 0.27 | 85,85,85,85                 | 0     |
| 85  | MG   | s8    | 301  | 1/1   | 0.71 | 0.27 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3648 | 1/1   | 0.71 | 0.30 | 72,72,72,72                 | 0     |
| 85  | MG   | 1     | 3733 | 1/1   | 0.71 | 0.19 | 46,46,46,46                 | 0     |
| 85  | MG   | 2     | 2019 | 1/1   | 0.71 | 0.37 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4174 | 7/7   | 0.71 | 0.30 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3448 | 1/1   | 0.71 | 0.23 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3651 | 1/1   | 0.72 | 0.23 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3711 | 1/1   | 0.72 | 0.23 | 52,52,52,52                 | 0     |
| 86  | OHX  | 2     | 2164 | 7/7   | 0.72 | 0.20 | 140,140,140,140             | 0     |
| 85  | MG   | 6     | 2039 | 1/1   | 0.72 | 0.43 | 67,67,67,67                 | 0     |
| 85  | MG   | 1     | 3631 | 1/1   | 0.72 | 0.36 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 1934 | 1/1   | 0.73 | 0.31 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 2003 | 1/1   | 0.73 | 0.20 | 60,60,60,60                 | 0     |
| 85  | MG   | M3    | 203  | 1/1   | 0.73 | 0.41 | 79,79,79,79                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1949 | 1/1   | 0.73 | 0.27 | 68,68,68,68                 | 0     |
| 85  | MG   | 2     | 1923 | 1/1   | 0.73 | 0.35 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3812 | 1/1   | 0.73 | 0.18 | 74,74,74,74                 | 0     |
| 86  | OHX  | 1     | 4189 | 7/7   | 0.73 | 0.22 | 145,145,145,145             | 0     |
| 85  | MG   | 2     | 1964 | 1/1   | 0.73 | 0.16 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3564 | 1/1   | 0.74 | 0.20 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1912 | 1/1   | 0.74 | 0.28 | 60,60,60,60                 | 0     |
| 85  | MG   | 3     | 214  | 1/1   | 0.74 | 0.27 | 50,50,50,50                 | 0     |
| 85  | MG   | 2     | 1994 | 1/1   | 0.74 | 0.23 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 4178 | 7/7   | 0.74 | 0.23 | 126,126,126,126             | 0     |
| 85  | MG   | 2     | 2020 | 1/1   | 0.74 | 0.42 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4229 | 7/7   | 0.74 | 0.22 | 131,131,131,131             | 0     |
| 86  | OHX  | 5     | 4234 | 7/7   | 0.74 | 0.26 | 111,111,111,111             | 0     |
| 85  | MG   | 2     | 2018 | 1/1   | 0.74 | 0.43 | 62,62,62,62                 | 0     |
| 87  | ZN   | D7    | 101  | 1/1   | 0.74 | 0.19 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3683 | 1/1   | 0.75 | 0.31 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 2035 | 1/1   | 0.75 | 0.42 | 74,74,74,74                 | 0     |
| 85  | MG   | 1     | 3402 | 1/1   | 0.75 | 0.36 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1983 | 1/1   | 0.75 | 0.31 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 1936 | 1/1   | 0.75 | 0.30 | 57,57,57,57                 | 0     |
| 85  | MG   | 6     | 1966 | 1/1   | 0.75 | 0.33 | 73,73,73,73                 | 0     |
| 85  | MG   | 6     | 1978 | 1/1   | 0.75 | 0.23 | 67,67,67,67                 | 0     |
| 85  | MG   | 1     | 3530 | 1/1   | 0.75 | 0.26 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 2005 | 1/1   | 0.75 | 0.29 | 81,81,81,81                 | 0     |
| 85  | MG   | 1     | 3865 | 1/1   | 0.75 | 0.42 | 67,67,67,67                 | 0     |
| 85  | MG   | 6     | 1923 | 1/1   | 0.75 | 0.27 | 56,56,56,56                 | 0     |
| 85  | MG   | 6     | 2030 | 1/1   | 0.75 | 0.25 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3679 | 1/1   | 0.76 | 0.08 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3844 | 1/1   | 0.76 | 0.18 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3854 | 1/1   | 0.76 | 0.34 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3767 | 1/1   | 0.76 | 0.14 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3456 | 1/1   | 0.76 | 0.37 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4202 | 7/7   | 0.76 | 0.25 | 110,110,110,110             | 0     |
| 86  | OHX  | L6    | 202  | 7/7   | 0.76 | 0.26 | 112,112,112,112             | 0     |
| 86  | OHX  | 5     | 4227 | 7/7   | 0.76 | 0.31 | 96,96,96,96                 | 0     |
| 85  | MG   | 2     | 1914 | 1/1   | 0.76 | 0.37 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 4230 | 7/7   | 0.76 | 0.28 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3886 | 1/1   | 0.76 | 0.47 | 80,80,80,80                 | 0     |
| 85  | MG   | 2     | 1997 | 1/1   | 0.76 | 0.31 | 80,80,80,80                 | 0     |
| 86  | OHX  | 5     | 4244 | 7/7   | 0.76 | 0.25 | 122,122,122,122             | 0     |
| 85  | MG   | 1     | 3835 | 1/1   | 0.76 | 0.29 | 46,46,46,46                 | 0     |
| 85  | MG   | s1    | 301  | 1/1   | 0.77 | 0.23 | 62,62,62,62                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3740 | 1/1   | 0.77 | 0.13 | 34,34,34,34                 | 0     |
| 85  | MG   | 3     | 202  | 1/1   | 0.77 | 0.18 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4190 | 7/7   | 0.77 | 0.24 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3499 | 1/1   | 0.77 | 0.29 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3864 | 1/1   | 0.77 | 0.14 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4205 | 7/7   | 0.77 | 0.26 | 113,113,113,113             | 0     |
| 85  | MG   | 6     | 1907 | 1/1   | 0.77 | 0.32 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3677 | 1/1   | 0.77 | 0.42 | 60,60,60,60                 | 0     |
| 86  | OHX  | 2     | 2160 | 7/7   | 0.77 | 0.23 | 117,117,117,117             | 0     |
| 86  | OHX  | 5     | 4233 | 7/7   | 0.77 | 0.23 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3568 | 1/1   | 0.77 | 0.27 | 23,23,23,23                 | 0     |
| 86  | OHX  | 2     | 2165 | 7/7   | 0.77 | 0.24 | 125,125,125,125             | 0     |
| 86  | OHX  | 2     | 2166 | 7/7   | 0.77 | 0.17 | 144,144,144,144             | 0     |
| 86  | OHX  | 14    | 403  | 7/7   | 0.77 | 0.26 | 111,111,111,111             | 0     |
| 86  | OHX  | 2     | 2178 | 7/7   | 0.77 | 0.20 | 141,141,141,141             | 0     |
| 85  | MG   | 4     | 221  | 1/1   | 0.78 | 0.39 | 45,45,45,45                 | 0     |
| 85  | MG   | 7     | 204  | 1/1   | 0.78 | 0.39 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4197 | 7/7   | 0.78 | 0.21 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3786 | 1/1   | 0.78 | 0.33 | 70,70,70,70                 | 0     |
| 85  | MG   | 2     | 1951 | 1/1   | 0.78 | 0.46 | 68,68,68,68                 | 0     |
| 86  | OHX  | M9    | 202  | 7/7   | 0.78 | 0.19 | 130,130,130,130             | 0     |
| 86  | OHX  | 6     | 2184 | 7/7   | 0.78 | 0.23 | 108,108,108,108             | 0     |
| 86  | OHX  | 6     | 2186 | 7/7   | 0.78 | 0.23 | 113,113,113,113             | 0     |
| 85  | MG   | 2     | 1928 | 1/1   | 0.78 | 0.40 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 4220 | 7/7   | 0.78 | 0.21 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3732 | 1/1   | 0.78 | 0.34 | 65,65,65,65                 | 0     |
| 85  | MG   | 6     | 1999 | 1/1   | 0.78 | 0.28 | 87,87,87,87                 | 0     |
| 85  | MG   | 6     | 1904 | 1/1   | 0.78 | 0.38 | 56,56,56,56                 | 0     |
| 85  | MG   | 2     | 1907 | 1/1   | 0.78 | 0.37 | 46,46,46,46                 | 0     |
| 86  | OHX  | 2     | 2179 | 7/7   | 0.78 | 0.19 | 137,137,137,137             | 0     |
| 86  | OHX  | 2     | 2181 | 7/7   | 0.78 | 0.22 | 130,130,130,130             | 0     |
| 86  | OHX  | 5     | 4240 | 7/7   | 0.78 | 0.14 | 192,192,192,192             | 0     |
| 86  | OHX  | 1     | 4144 | 7/7   | 0.78 | 0.26 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3780 | 1/1   | 0.78 | 0.35 | 70,70,70,70                 | 0     |
| 85  | MG   | 5     | 3895 | 1/1   | 0.78 | 0.25 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4192 | 7/7   | 0.79 | 0.29 | 98,98,98,98                 | 0     |
| 85  | MG   | 2     | 1950 | 1/1   | 0.79 | 0.22 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3787 | 1/1   | 0.79 | 0.18 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3590 | 1/1   | 0.79 | 0.35 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3490 | 1/1   | 0.79 | 0.20 | 51,51,51,51                 | 0     |
| 86  | OHX  | 2     | 2161 | 7/7   | 0.79 | 0.24 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3602 | 1/1   | 0.79 | 0.18 | 40,40,40,40                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 6     | 2190 | 7/7   | 0.79 | 0.24 | 110,110,110,110             | 0     |
| 86  | OHX  | 6     | 2193 | 7/7   | 0.79 | 0.18 | 142,142,142,142             | 0     |
| 86  | OHX  | 6     | 2196 | 7/7   | 0.79 | 0.17 | 142,142,142,142             | 0     |
| 85  | MG   | 1     | 3707 | 1/1   | 0.79 | 0.10 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4212 | 7/7   | 0.79 | 0.28 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3495 | 1/1   | 0.79 | 0.21 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3654 | 1/1   | 0.79 | 0.08 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 2031 | 1/1   | 0.79 | 0.28 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3840 | 1/1   | 0.79 | 0.28 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4142 | 7/7   | 0.79 | 0.31 | 89,89,89,89                 | 0     |
| 85  | MG   | 4     | 211  | 1/1   | 0.79 | 0.23 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3426 | 1/1   | 0.79 | 0.14 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3734 | 1/1   | 0.79 | 0.25 | 68,68,68,68                 | 0     |
| 86  | OHX  | 1     | 4188 | 7/7   | 0.79 | 0.23 | 115,115,115,115             | 0     |
| 86  | OHX  | 7     | 227  | 7/7   | 0.79 | 0.19 | 127,127,127,127             | 0     |
| 85  | MG   | 2     | 1976 | 1/1   | 0.79 | 0.28 | 43,43,43,43                 | 0     |
| 86  | OHX  | m1    | 203  | 7/7   | 0.79 | 0.21 | 124,124,124,124             | 0     |
| 85  | MG   | 6     | 1984 | 1/1   | 0.79 | 0.17 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3626 | 1/1   | 0.80 | 0.17 | 39,39,39,39                 | 0     |
| 86  | OHX  | 6     | 2185 | 7/7   | 0.80 | 0.16 | 143,143,143,143             | 0     |
| 85  | MG   | 2     | 2002 | 1/1   | 0.80 | 0.22 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3636 | 1/1   | 0.80 | 0.15 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3667 | 1/1   | 0.80 | 0.12 | 31,31,31,31                 | 0     |
| 85  | MG   | 2     | 2183 | 1/1   | 0.80 | 0.34 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 4163 | 7/7   | 0.80 | 0.18 | 145,145,145,145             | 0     |
| 85  | MG   | 1     | 3782 | 1/1   | 0.80 | 0.15 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3852 | 1/1   | 0.80 | 0.13 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4219 | 7/7   | 0.80 | 0.24 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3875 | 1/1   | 0.80 | 0.29 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4224 | 7/7   | 0.80 | 0.21 | 113,113,113,113             | 0     |
| 85  | MG   | S8    | 301  | 1/1   | 0.80 | 0.19 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1978 | 1/1   | 0.80 | 0.27 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 4180 | 7/7   | 0.80 | 0.21 | 120,120,120,120             | 0     |
| 86  | OHX  | 1     | 4183 | 7/7   | 0.80 | 0.24 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 2013 | 1/1   | 0.80 | 0.10 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1961 | 1/1   | 0.80 | 0.23 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 4238 | 7/7   | 0.80 | 0.23 | 117,117,117,117             | 0     |
| 86  | OHX  | 5     | 4239 | 7/7   | 0.80 | 0.19 | 149,149,149,149             | 0     |
| 85  | MG   | 5     | 3500 | 1/1   | 0.80 | 0.15 | 45,45,45,45                 | 0     |
| 85  | MG   | 2     | 1926 | 1/1   | 0.80 | 0.41 | 77,77,77,77                 | 0     |
| 85  | MG   | 5     | 3600 | 1/1   | 0.80 | 0.12 | 50,50,50,50                 | 0     |
| 85  | MG   | o1    | 201  | 1/1   | 0.80 | 0.12 | 76,76,76,76                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1930 | 1/1   | 0.80 | 0.23 | 53,53,53,53                 | 0     |
| 86  | OHX  | m4    | 202  | 7/7   | 0.80 | 0.14 | 190,190,190,190             | 0     |
| 85  | MG   | 2     | 1946 | 1/1   | 0.80 | 0.36 | 64,64,64,64                 | 0     |
| 85  | MG   | 6     | 1939 | 1/1   | 0.81 | 0.33 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 1963 | 1/1   | 0.81 | 0.25 | 67,67,67,67                 | 0     |
| 86  | OHX  | M7    | 208  | 7/7   | 0.81 | 0.24 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3655 | 1/1   | 0.81 | 0.16 | 25,25,25,25                 | 0     |
| 86  | OHX  | 6     | 2181 | 7/7   | 0.81 | 0.24 | 113,113,113,113             | 0     |
| 85  | MG   | 6     | 1968 | 1/1   | 0.81 | 0.34 | 65,65,65,65                 | 0     |
| 85  | MG   | 8     | 209  | 1/1   | 0.81 | 0.24 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3624 | 1/1   | 0.81 | 0.43 | 69,69,69,69                 | 0     |
| 86  | OHX  | 6     | 2188 | 7/7   | 0.81 | 0.21 | 120,120,120,120             | 0     |
| 85  | MG   | 2     | 1924 | 1/1   | 0.81 | 0.42 | 65,65,65,65                 | 0     |
| 86  | OHX  | 2     | 2159 | 7/7   | 0.81 | 0.12 | 260,260,260,260             | 0     |
| 85  | MG   | 5     | 3756 | 1/1   | 0.81 | 0.14 | 36,36,36,36                 | 0     |
| 86  | OHX  | 6     | 2204 | 7/7   | 0.81 | 0.20 | 118,118,118,118             | 0     |
| 85  | MG   | N0    | 201  | 1/1   | 0.81 | 0.27 | 42,42,42,42                 | 0     |
| 86  | OHX  | 5     | 4186 | 7/7   | 0.81 | 0.21 | 120,120,120,120             | 0     |
| 86  | OHX  | 5     | 4204 | 7/7   | 0.81 | 0.23 | 111,111,111,111             | 0     |
| 86  | OHX  | 2     | 2163 | 7/7   | 0.81 | 0.18 | 138,138,138,138             | 0     |
| 85  | MG   | 5     | 3469 | 1/1   | 0.81 | 0.24 | 101,101,101,101             | 0     |
| 85  | MG   | 5     | 3477 | 1/1   | 0.81 | 0.32 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3808 | 1/1   | 0.81 | 0.17 | 30,30,30,30                 | 0     |
| 85  | MG   | 2     | 1905 | 1/1   | 0.81 | 0.35 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3789 | 1/1   | 0.81 | 0.19 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3819 | 1/1   | 0.81 | 0.08 | 42,42,42,42                 | 0     |
| 85  | MG   | 3     | 201  | 1/1   | 0.81 | 0.35 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3801 | 1/1   | 0.81 | 0.18 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4167 | 7/7   | 0.81 | 0.24 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4173 | 7/7   | 0.81 | 0.20 | 132,132,132,132             | 0     |
| 85  | MG   | 5     | 3605 | 1/1   | 0.81 | 0.25 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3465 | 1/1   | 0.81 | 0.24 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3818 | 1/1   | 0.81 | 0.09 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 2029 | 1/1   | 0.81 | 0.51 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3821 | 1/1   | 0.81 | 0.10 | 37,37,37,37                 | 0     |
| 86  | OHX  | 8     | 225  | 7/7   | 0.81 | 0.21 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3475 | 1/1   | 0.81 | 0.26 | 64,64,64,64                 | 0     |
| 86  | OHX  | l5    | 306  | 7/7   | 0.81 | 0.21 | 114,114,114,114             | 0     |
| 85  | MG   | 2     | 1931 | 1/1   | 0.81 | 0.33 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3493 | 1/1   | 0.81 | 0.34 | 69,69,69,69                 | 0     |
| 86  | OHX  | m8    | 201  | 7/7   | 0.81 | 0.24 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3893 | 1/1   | 0.81 | 0.12 | 95,95,95,95                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 8     | 206  | 1/1   | 0.82 | 0.17 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3767 | 1/1   | 0.82 | 0.10 | 29,29,29,29                 | 0     |
| 86  | OHX  | O9    | 101  | 7/7   | 0.82 | 0.27 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3479 | 1/1   | 0.82 | 0.30 | 56,56,56,56                 | 0     |
| 86  | OHX  | 6     | 2183 | 7/7   | 0.82 | 0.20 | 118,118,118,118             | 0     |
| 85  | MG   | 1     | 3687 | 1/1   | 0.82 | 0.33 | 69,69,69,69                 | 0     |
| 85  | MG   | 6     | 1952 | 1/1   | 0.82 | 0.34 | 53,53,53,53                 | 0     |
| 85  | MG   | 6     | 1958 | 1/1   | 0.82 | 0.36 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3828 | 1/1   | 0.82 | 0.09 | 35,35,35,35                 | 0     |
| 86  | OHX  | 6     | 2189 | 7/7   | 0.82 | 0.22 | 115,115,115,115             | 0     |
| 85  | MG   | 6     | 2034 | 1/1   | 0.82 | 0.23 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3636 | 1/1   | 0.82 | 0.10 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3616 | 1/1   | 0.82 | 0.14 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3479 | 1/1   | 0.82 | 0.32 | 70,70,70,70                 | 0     |
| 85  | MG   | 6     | 1970 | 1/1   | 0.82 | 0.13 | 49,49,49,49                 | 0     |
| 85  | MG   | 6     | 2045 | 1/1   | 0.82 | 0.41 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3470 | 1/1   | 0.82 | 0.19 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3731 | 1/1   | 0.82 | 0.11 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3401 | 1/1   | 0.82 | 0.26 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4217 | 7/7   | 0.82 | 0.23 | 106,106,106,106             | 0     |
| 85  | MG   | 5     | 3856 | 1/1   | 0.82 | 0.43 | 68,68,68,68                 | 0     |
| 86  | OHX  | 1     | 4169 | 7/7   | 0.82 | 0.28 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3865 | 1/1   | 0.82 | 0.17 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4226 | 7/7   | 0.82 | 0.19 | 130,130,130,130             | 0     |
| 85  | MG   | 5     | 3866 | 1/1   | 0.82 | 0.08 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3853 | 1/1   | 0.82 | 0.16 | 35,35,35,35                 | 0     |
| 86  | OHX  | 1     | 4179 | 7/7   | 0.82 | 0.28 | 101,101,101,101             | 0     |
| 85  | MG   | 4     | 204  | 1/1   | 0.82 | 0.34 | 60,60,60,60                 | 0     |
| 85  | MG   | 2     | 1990 | 1/1   | 0.82 | 0.34 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4185 | 7/7   | 0.82 | 0.22 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3887 | 1/1   | 0.82 | 0.40 | 53,53,53,53                 | 0     |
| 85  | MG   | 6     | 2007 | 1/1   | 0.82 | 0.14 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3611 | 1/1   | 0.82 | 0.09 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4191 | 7/7   | 0.82 | 0.24 | 104,104,104,104             | 0     |
| 86  | OHX  | 5     | 4246 | 7/7   | 0.82 | 0.20 | 122,122,122,122             | 0     |
| 86  | OHX  | 7     | 225  | 7/7   | 0.82 | 0.21 | 118,118,118,118             | 0     |
| 85  | MG   | 1     | 3752 | 1/1   | 0.82 | 0.24 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3762 | 1/1   | 0.82 | 0.19 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 4199 | 7/7   | 0.82 | 0.25 | 107,107,107,107             | 0     |
| 86  | OHX  | 1     | 4200 | 7/7   | 0.82 | 0.22 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3765 | 1/1   | 0.82 | 0.12 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4205 | 7/7   | 0.82 | 0.22 | 108,108,108,108             | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 4     | 236  | 7/7   | 0.82 | 0.26 | 105,105,105,105             | 0     |
| 85  | MG   | 7     | 215  | 1/1   | 0.82 | 0.31 | 48,48,48,48                 | 0     |
| 86  | OHX  | 6     | 2170 | 7/7   | 0.83 | 0.20 | 117,117,117,117             | 0     |
| 86  | OHX  | 6     | 2178 | 7/7   | 0.83 | 0.20 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3407 | 1/1   | 0.83 | 0.17 | 34,34,34,34                 | 0     |
| 86  | OHX  | 2     | 2173 | 7/7   | 0.83 | 0.21 | 121,121,121,121             | 0     |
| 85  | MG   | 1     | 3411 | 1/1   | 0.83 | 0.18 | 33,33,33,33                 | 0     |
| 85  | MG   | 6     | 1967 | 1/1   | 0.83 | 0.20 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3824 | 1/1   | 0.83 | 0.10 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4130 | 7/7   | 0.83 | 0.19 | 120,120,120,120             | 0     |
| 85  | MG   | 2     | 1934 | 1/1   | 0.83 | 0.32 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3713 | 1/1   | 0.83 | 0.51 | 73,73,73,73                 | 0     |
| 86  | OHX  | 1     | 4162 | 7/7   | 0.83 | 0.19 | 121,121,121,121             | 0     |
| 86  | OHX  | 6     | 2195 | 7/7   | 0.83 | 0.19 | 127,127,127,127             | 0     |
| 85  | MG   | 1     | 3721 | 1/1   | 0.83 | 0.31 | 44,44,44,44                 | 0     |
| 86  | OHX  | 6     | 2203 | 7/7   | 0.83 | 0.21 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3884 | 1/1   | 0.83 | 0.39 | 55,55,55,55                 | 0     |
| 86  | OHX  | c3    | 201  | 7/7   | 0.83 | 0.19 | 122,122,122,122             | 0     |
| 86  | OHX  | 1     | 4172 | 7/7   | 0.83 | 0.18 | 123,123,123,123             | 0     |
| 85  | MG   | 5     | 3429 | 1/1   | 0.83 | 0.34 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4190 | 7/7   | 0.83 | 0.25 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4193 | 7/7   | 0.83 | 0.25 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4203 | 7/7   | 0.83 | 0.22 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 1987 | 1/1   | 0.83 | 0.17 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3639 | 1/1   | 0.83 | 0.12 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3894 | 1/1   | 0.83 | 0.31 | 45,45,45,45                 | 0     |
| 85  | MG   | 2     | 1939 | 1/1   | 0.83 | 0.28 | 57,57,57,57                 | 0     |
| 86  | OHX  | 5     | 4218 | 7/7   | 0.83 | 0.16 | 141,141,141,141             | 0     |
| 85  | MG   | 1     | 3607 | 1/1   | 0.83 | 0.27 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3738 | 1/1   | 0.83 | 0.16 | 24,24,24,24                 | 0     |
| 86  | OHX  | 5     | 4223 | 7/7   | 0.83 | 0.21 | 117,117,117,117             | 0     |
| 86  | OHX  | 1     | 4187 | 7/7   | 0.83 | 0.25 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3484 | 1/1   | 0.83 | 0.27 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1904 | 1/1   | 0.83 | 0.46 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3550 | 1/1   | 0.83 | 0.17 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3615 | 1/1   | 0.83 | 0.20 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3659 | 1/1   | 0.83 | 0.16 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 4195 | 7/7   | 0.83 | 0.19 | 116,116,116,116             | 0     |
| 85  | MG   | 1     | 3663 | 1/1   | 0.83 | 0.11 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4198 | 7/7   | 0.83 | 0.18 | 125,125,125,125             | 0     |
| 85  | MG   | o4    | 202  | 1/1   | 0.83 | 0.31 | 50,50,50,50                 | 0     |
| 86  | OHX  | 2     | 2125 | 7/7   | 0.83 | 0.19 | 120,120,120,120             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2146 | 7/7   | 0.83 | 0.20 | 115,115,115,115             | 0     |
| 86  | OHX  | 1     | 4204 | 7/7   | 0.83 | 0.24 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3666 | 1/1   | 0.83 | 0.10 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 4211 | 7/7   | 0.83 | 0.26 | 106,106,106,106             | 0     |
| 86  | OHX  | 4     | 234  | 7/7   | 0.83 | 0.21 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3630 | 1/1   | 0.83 | 0.46 | 75,75,75,75                 | 0     |
| 85  | MG   | 1     | 3672 | 1/1   | 0.83 | 0.16 | 36,36,36,36                 | 0     |
| 85  | MG   | 3     | 203  | 1/1   | 0.83 | 0.25 | 75,75,75,75                 | 0     |
| 85  | MG   | 2     | 1948 | 1/1   | 0.83 | 0.43 | 57,57,57,57                 | 0     |
| 85  | MG   | 2     | 1987 | 1/1   | 0.83 | 0.27 | 91,91,91,91                 | 0     |
| 86  | OHX  | 6     | 2148 | 7/7   | 0.83 | 0.19 | 108,108,108,108             | 0     |
| 86  | OHX  | 1     | 4203 | 7/7   | 0.84 | 0.23 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3672 | 1/1   | 0.84 | 0.16 | 57,57,57,57                 | 0     |
| 85  | MG   | 2     | 1965 | 1/1   | 0.84 | 0.30 | 74,74,74,74                 | 0     |
| 85  | MG   | 7     | 214  | 1/1   | 0.84 | 0.25 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 4214 | 7/7   | 0.84 | 0.24 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4215 | 7/7   | 0.84 | 0.22 | 118,118,118,118             | 0     |
| 85  | MG   | 6     | 1910 | 1/1   | 0.84 | 0.24 | 54,54,54,54                 | 0     |
| 86  | OHX  | 4     | 235  | 7/7   | 0.84 | 0.21 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3696 | 1/1   | 0.84 | 0.18 | 36,36,36,36                 | 0     |
| 86  | OHX  | L3    | 404  | 7/7   | 0.84 | 0.19 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3852 | 1/1   | 0.84 | 0.17 | 43,43,43,43                 | 0     |
| 86  | OHX  | M7    | 207  | 7/7   | 0.84 | 0.30 | 83,83,83,83                 | 0     |
| 85  | MG   | l5    | 303  | 1/1   | 0.84 | 0.19 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 1915 | 1/1   | 0.84 | 0.23 | 57,57,57,57                 | 0     |
| 85  | MG   | 1     | 3417 | 1/1   | 0.84 | 0.27 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3731 | 1/1   | 0.84 | 0.10 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2116 | 7/7   | 0.84 | 0.20 | 111,111,111,111             | 0     |
| 85  | MG   | 1     | 3732 | 1/1   | 0.84 | 0.13 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2138 | 7/7   | 0.84 | 0.17 | 132,132,132,132             | 0     |
| 86  | OHX  | 2     | 2144 | 7/7   | 0.84 | 0.23 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3737 | 1/1   | 0.84 | 0.14 | 36,36,36,36                 | 0     |
| 86  | OHX  | 2     | 2157 | 7/7   | 0.84 | 0.14 | 195,195,195,195             | 0     |
| 85  | MG   | 5     | 3738 | 1/1   | 0.84 | 0.35 | 61,61,61,61                 | 0     |
| 86  | OHX  | 6     | 2187 | 7/7   | 0.84 | 0.16 | 136,136,136,136             | 0     |
| 85  | MG   | 6     | 2041 | 1/1   | 0.84 | 0.47 | 65,65,65,65                 | 0     |
| 85  | MG   | 6     | 1933 | 1/1   | 0.84 | 0.37 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3761 | 1/1   | 0.84 | 0.22 | 64,64,64,64                 | 0     |
| 86  | OHX  | 6     | 2191 | 7/7   | 0.84 | 0.19 | 131,131,131,131             | 0     |
| 86  | OHX  | 6     | 2192 | 7/7   | 0.84 | 0.18 | 130,130,130,130             | 0     |
| 85  | MG   | 2     | 1910 | 1/1   | 0.84 | 0.30 | 48,48,48,48                 | 0     |
| 85  | MG   | 2     | 1999 | 1/1   | 0.84 | 0.10 | 83,83,83,83                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1929 | 1/1   | 0.84 | 0.34 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3769 | 1/1   | 0.84 | 0.14 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2176 | 7/7   | 0.84 | 0.20 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3412 | 1/1   | 0.84 | 0.12 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4145 | 7/7   | 0.84 | 0.24 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 4159 | 7/7   | 0.84 | 0.22 | 101,101,101,101             | 0     |
| 85  | MG   | 6     | 1941 | 1/1   | 0.84 | 0.20 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4181 | 7/7   | 0.84 | 0.20 | 107,107,107,107             | 0     |
| 86  | OHX  | 2     | 2180 | 7/7   | 0.84 | 0.21 | 116,116,116,116             | 0     |
| 85  | MG   | 1     | 3447 | 1/1   | 0.84 | 0.27 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4066 | 7/7   | 0.84 | 0.23 | 106,106,106,106             | 0     |
| 86  | OHX  | 5     | 4194 | 7/7   | 0.84 | 0.19 | 116,116,116,116             | 0     |
| 86  | OHX  | 5     | 4200 | 7/7   | 0.84 | 0.19 | 114,114,114,114             | 0     |
| 86  | OHX  | 5     | 4202 | 7/7   | 0.84 | 0.22 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3547 | 1/1   | 0.84 | 0.11 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 4135 | 7/7   | 0.84 | 0.24 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 4141 | 7/7   | 0.84 | 0.21 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3548 | 1/1   | 0.84 | 0.33 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1952 | 1/1   | 0.84 | 0.38 | 75,75,75,75                 | 0     |
| 86  | OHX  | 1     | 4148 | 7/7   | 0.84 | 0.20 | 118,118,118,118             | 0     |
| 86  | OHX  | 1     | 4152 | 7/7   | 0.84 | 0.18 | 124,124,124,124             | 0     |
| 85  | MG   | 1     | 3566 | 1/1   | 0.84 | 0.33 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3801 | 1/1   | 0.84 | 0.11 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3462 | 1/1   | 0.84 | 0.17 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3464 | 1/1   | 0.84 | 0.10 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3805 | 1/1   | 0.84 | 0.19 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3489 | 1/1   | 0.84 | 0.13 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3814 | 1/1   | 0.84 | 0.22 | 53,53,53,53                 | 0     |
| 85  | MG   | 6     | 1981 | 1/1   | 0.84 | 0.21 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3837 | 1/1   | 0.84 | 0.16 | 40,40,40,40                 | 0     |
| 85  | MG   | 2     | 2005 | 1/1   | 0.84 | 0.17 | 59,59,59,59                 | 0     |
| 85  | MG   | 4     | 216  | 1/1   | 0.84 | 0.13 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3578 | 1/1   | 0.84 | 0.21 | 28,28,28,28                 | 0     |
| 85  | MG   | 6     | 1992 | 1/1   | 0.84 | 0.12 | 40,40,40,40                 | 0     |
| 85  | MG   | 2     | 1963 | 1/1   | 0.84 | 0.29 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 4245 | 7/7   | 0.84 | 0.22 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3696 | 1/1   | 0.84 | 0.12 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4247 | 7/7   | 0.84 | 0.22 | 102,102,102,102             | 0     |
| 85  | MG   | 5     | 3627 | 1/1   | 0.84 | 0.24 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3700 | 1/1   | 0.84 | 0.11 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4193 | 7/7   | 0.84 | 0.22 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3471 | 1/1   | 0.84 | 0.12 | 35,35,35,35                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1941 | 1/1   | 0.84 | 0.21 | 50,50,50,50                 | 0     |
| 85  | MG   | N8    | 201  | 1/1   | 0.84 | 0.10 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3622 | 1/1   | 0.84 | 0.21 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 2027 | 1/1   | 0.84 | 0.26 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3478 | 1/1   | 0.84 | 0.17 | 36,36,36,36                 | 0     |
| 87  | ZN   | d7    | 101  | 1/1   | 0.84 | 0.21 | 119,119,119,119             | 0     |
| 86  | OHX  | 1     | 4182 | 7/7   | 0.85 | 0.22 | 106,106,106,106             | 0     |
| 85  | MG   | 4     | 219  | 1/1   | 0.85 | 0.18 | 45,45,45,45                 | 0     |
| 86  | OHX  | 6     | 2194 | 7/7   | 0.85 | 0.16 | 140,140,140,140             | 0     |
| 86  | OHX  | 1     | 4184 | 7/7   | 0.85 | 0.25 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2141 | 7/7   | 0.85 | 0.18 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3855 | 1/1   | 0.85 | 0.19 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 1975 | 1/1   | 0.85 | 0.27 | 53,53,53,53                 | 0     |
| 86  | OHX  | s9    | 201  | 7/7   | 0.85 | 0.22 | 102,102,102,102             | 0     |
| 86  | OHX  | 2     | 2150 | 7/7   | 0.85 | 0.16 | 134,134,134,134             | 0     |
| 86  | OHX  | 5     | 4139 | 7/7   | 0.85 | 0.23 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3422 | 1/1   | 0.85 | 0.24 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 4146 | 7/7   | 0.85 | 0.23 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3424 | 1/1   | 0.85 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3872 | 1/1   | 0.85 | 0.27 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3873 | 1/1   | 0.85 | 0.40 | 47,47,47,47                 | 0     |
| 86  | OHX  | 2     | 2162 | 7/7   | 0.85 | 0.19 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3640 | 1/1   | 0.85 | 0.11 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3751 | 1/1   | 0.85 | 0.12 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3708 | 1/1   | 0.85 | 0.15 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3480 | 1/1   | 0.85 | 0.27 | 57,57,57,57                 | 0     |
| 86  | OHX  | 2     | 2170 | 7/7   | 0.85 | 0.20 | 126,126,126,126             | 0     |
| 85  | MG   | 1     | 3488 | 1/1   | 0.85 | 0.13 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3888 | 1/1   | 0.85 | 0.14 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3769 | 1/1   | 0.85 | 0.24 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 4209 | 7/7   | 0.85 | 0.24 | 91,91,91,91                 | 0     |
| 86  | OHX  | 1     | 4206 | 7/7   | 0.85 | 0.22 | 106,106,106,106             | 0     |
| 86  | OHX  | 5     | 4214 | 7/7   | 0.85 | 0.22 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3478 | 1/1   | 0.85 | 0.28 | 50,50,50,50                 | 0     |
| 85  | MG   | 2     | 1996 | 1/1   | 0.85 | 0.41 | 48,48,48,48                 | 0     |
| 85  | MG   | 2     | 1959 | 1/1   | 0.85 | 0.46 | 66,66,66,66                 | 0     |
| 86  | OHX  | 3     | 224  | 7/7   | 0.85 | 0.17 | 132,132,132,132             | 0     |
| 86  | OHX  | 5     | 4222 | 7/7   | 0.85 | 0.25 | 101,101,101,101             | 0     |
| 85  | MG   | 5     | 3897 | 1/1   | 0.85 | 0.18 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3689 | 1/1   | 0.85 | 0.13 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4134 | 7/7   | 0.85 | 0.19 | 127,127,127,127             | 0     |
| 85  | MG   | 6     | 2042 | 1/1   | 0.85 | 0.39 | 65,65,65,65                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85  | MG   | 5     | 3701 | 1/1   | 0.85 | 0.20 | 56,56,56,56                | 0     |
| 85  | MG   | 1     | 3790 | 1/1   | 0.85 | 0.10 | 33,33,33,33                | 0     |
| 85  | MG   | 8     | 202  | 1/1   | 0.85 | 0.12 | 47,47,47,47                | 0     |
| 86  | OHX  | 1     | 4147 | 7/7   | 0.85 | 0.20 | 120,120,120,120            | 0     |
| 86  | OHX  | 5     | 4235 | 7/7   | 0.85 | 0.25 | 106,106,106,106            | 0     |
| 85  | MG   | 8     | 205  | 1/1   | 0.85 | 0.13 | 59,59,59,59                | 0     |
| 86  | OHX  | 6     | 2136 | 7/7   | 0.85 | 0.22 | 105,105,105,105            | 0     |
| 85  | MG   | 5     | 3527 | 1/1   | 0.85 | 0.11 | 26,26,26,26                | 0     |
| 86  | OHX  | 6     | 2165 | 7/7   | 0.85 | 0.19 | 119,119,119,119            | 0     |
| 85  | MG   | 2     | 1909 | 1/1   | 0.85 | 0.35 | 59,59,59,59                | 0     |
| 86  | OHX  | 6     | 2174 | 7/7   | 0.85 | 0.24 | 101,101,101,101            | 0     |
| 86  | OHX  | 1     | 4166 | 7/7   | 0.85 | 0.18 | 130,130,130,130            | 0     |
| 86  | OHX  | 6     | 2179 | 7/7   | 0.85 | 0.17 | 123,123,123,123            | 0     |
| 86  | OHX  | 5     | 4248 | 7/7   | 0.85 | 0.19 | 126,126,126,126            | 0     |
| 85  | MG   | 1     | 3406 | 1/1   | 0.85 | 0.10 | 26,26,26,26                | 0     |
| 85  | MG   | n6    | 201  | 1/1   | 0.85 | 0.16 | 52,52,52,52                | 0     |
| 86  | OHX  | 1     | 4171 | 7/7   | 0.85 | 0.25 | 91,91,91,91                | 0     |
| 85  | MG   | 5     | 3816 | 1/1   | 0.85 | 0.13 | 37,37,37,37                | 0     |
| 85  | MG   | c7    | 201  | 1/1   | 0.85 | 0.37 | 63,63,63,63                | 0     |
| 85  | MG   | 5     | 3822 | 1/1   | 0.85 | 0.26 | 78,78,78,78                | 0     |
| 86  | OHX  | 1     | 4177 | 7/7   | 0.85 | 0.19 | 114,114,114,114            | 0     |
| 85  | MG   | 1     | 3592 | 1/1   | 0.85 | 0.33 | 43,43,43,43                | 0     |
| 86  | OHX  | 2     | 2120 | 7/7   | 0.85 | 0.19 | 111,111,111,111            | 0     |
| 85  | MG   | 1     | 3528 | 1/1   | 0.85 | 0.25 | 37,37,37,37                | 0     |
| 86  | OHX  | 1     | 4116 | 7/7   | 0.86 | 0.27 | 91,91,91,91                | 0     |
| 85  | MG   | 4     | 202  | 1/1   | 0.86 | 0.26 | 48,48,48,48                | 0     |
| 86  | OHX  | 6     | 2175 | 7/7   | 0.86 | 0.19 | 122,122,122,122            | 0     |
| 86  | OHX  | 1     | 4132 | 7/7   | 0.86 | 0.16 | 129,129,129,129            | 0     |
| 86  | OHX  | 1     | 4133 | 7/7   | 0.86 | 0.19 | 121,121,121,121            | 0     |
| 85  | MG   | 1     | 3421 | 1/1   | 0.86 | 0.24 | 37,37,37,37                | 0     |
| 85  | MG   | 2     | 2008 | 1/1   | 0.86 | 0.36 | 40,40,40,40                | 0     |
| 86  | OHX  | 1     | 4136 | 7/7   | 0.86 | 0.21 | 106,106,106,106            | 0     |
| 86  | OHX  | 1     | 4138 | 7/7   | 0.86 | 0.23 | 91,91,91,91                | 0     |
| 85  | MG   | 5     | 3880 | 1/1   | 0.86 | 0.25 | 45,45,45,45                | 0     |
| 85  | MG   | 5     | 3691 | 1/1   | 0.86 | 0.14 | 38,38,38,38                | 0     |
| 85  | MG   | 1     | 3542 | 1/1   | 0.86 | 0.28 | 27,27,27,27                | 0     |
| 86  | OHX  | 1     | 4145 | 7/7   | 0.86 | 0.18 | 110,110,110,110            | 0     |
| 86  | OHX  | 1     | 4146 | 7/7   | 0.86 | 0.24 | 94,94,94,94                | 0     |
| 85  | MG   | 1     | 3634 | 1/1   | 0.86 | 0.33 | 60,60,60,60                | 0     |
| 85  | MG   | 5     | 3702 | 1/1   | 0.86 | 0.11 | 44,44,44,44                | 0     |
| 85  | MG   | 1     | 3546 | 1/1   | 0.86 | 0.28 | 52,52,52,52                | 0     |
| 85  | MG   | 6     | 1972 | 1/1   | 0.86 | 0.11 | 46,46,46,46                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3427 | 1/1   | 0.86 | 0.17 | 27,27,27,27                 | 0     |
| 85  | MG   | L3    | 402  | 1/1   | 0.86 | 0.15 | 43,43,43,43                 | 0     |
| 86  | OHX  | 6     | 2199 | 7/7   | 0.86 | 0.21 | 110,110,110,110             | 0     |
| 86  | OHX  | 6     | 2200 | 7/7   | 0.86 | 0.21 | 115,115,115,115             | 0     |
| 86  | OHX  | 1     | 4168 | 7/7   | 0.86 | 0.13 | 161,161,161,161             | 0     |
| 85  | MG   | L5    | 301  | 1/1   | 0.86 | 0.35 | 50,50,50,50                 | 0     |
| 86  | OHX  | s1    | 303  | 7/7   | 0.86 | 0.18 | 128,128,128,128             | 0     |
| 86  | OHX  | 1     | 4170 | 7/7   | 0.86 | 0.23 | 95,95,95,95                 | 0     |
| 85  | MG   | 5     | 3455 | 1/1   | 0.86 | 0.21 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 4109 | 7/7   | 0.86 | 0.29 | 93,93,93,93                 | 0     |
| 85  | MG   | 2     | 1980 | 1/1   | 0.86 | 0.19 | 55,55,55,55                 | 0     |
| 85  | MG   | 6     | 1986 | 1/1   | 0.86 | 0.08 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3742 | 1/1   | 0.86 | 0.14 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4151 | 7/7   | 0.86 | 0.25 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 4152 | 7/7   | 0.86 | 0.25 | 95,95,95,95                 | 0     |
| 85  | MG   | 5     | 3746 | 1/1   | 0.86 | 0.28 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 4162 | 7/7   | 0.86 | 0.20 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3474 | 1/1   | 0.86 | 0.29 | 64,64,64,64                 | 0     |
| 86  | OHX  | 5     | 4164 | 7/7   | 0.86 | 0.20 | 111,111,111,111             | 0     |
| 86  | OHX  | 5     | 4174 | 7/7   | 0.86 | 0.22 | 109,109,109,109             | 0     |
| 85  | MG   | M3    | 204  | 1/1   | 0.86 | 0.09 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3553 | 1/1   | 0.86 | 0.17 | 46,46,46,46                 | 0     |
| 85  | MG   | 8     | 208  | 1/1   | 0.86 | 0.12 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3764 | 1/1   | 0.86 | 0.16 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3554 | 1/1   | 0.86 | 0.19 | 21,21,21,21                 | 0     |
| 86  | OHX  | 5     | 4195 | 7/7   | 0.86 | 0.24 | 95,95,95,95                 | 0     |
| 85  | MG   | 6     | 2000 | 1/1   | 0.86 | 0.15 | 42,42,42,42                 | 0     |
| 86  | OHX  | 5     | 4201 | 7/7   | 0.86 | 0.24 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3485 | 1/1   | 0.86 | 0.12 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3560 | 1/1   | 0.86 | 0.28 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3494 | 1/1   | 0.86 | 0.11 | 23,23,23,23                 | 0     |
| 85  | MG   | q1    | 101  | 1/1   | 0.86 | 0.20 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3776 | 1/1   | 0.86 | 0.23 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 4210 | 7/7   | 0.86 | 0.21 | 109,109,109,109             | 0     |
| 86  | OHX  | 5     | 4211 | 7/7   | 0.86 | 0.19 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3496 | 1/1   | 0.86 | 0.17 | 39,39,39,39                 | 0     |
| 85  | MG   | 2     | 2012 | 1/1   | 0.86 | 0.35 | 57,57,57,57                 | 0     |
| 85  | MG   | 5     | 3782 | 1/1   | 0.86 | 0.13 | 64,64,64,64                 | 0     |
| 86  | OHX  | 2     | 2140 | 7/7   | 0.86 | 0.19 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3503 | 1/1   | 0.86 | 0.27 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3858 | 1/1   | 0.86 | 0.23 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3484 | 1/1   | 0.86 | 0.32 | 38,38,38,38                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3566 | 1/1   | 0.86 | 0.28 | 24,24,24,24                 | 0     |
| 85  | MG   | 2     | 1944 | 1/1   | 0.86 | 0.14 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 4225 | 7/7   | 0.86 | 0.22 | 105,105,105,105             | 0     |
| 85  | MG   | 2     | 1945 | 1/1   | 0.86 | 0.20 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1919 | 1/1   | 0.86 | 0.37 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 1920 | 1/1   | 0.86 | 0.38 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 4207 | 7/7   | 0.86 | 0.23 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 4210 | 7/7   | 0.86 | 0.25 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3686 | 1/1   | 0.86 | 0.20 | 44,44,44,44                 | 0     |
| 85  | MG   | 2     | 1977 | 1/1   | 0.86 | 0.27 | 73,73,73,73                 | 0     |
| 85  | MG   | 6     | 1930 | 1/1   | 0.86 | 0.17 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4237 | 7/7   | 0.86 | 0.17 | 116,116,116,116             | 0     |
| 85  | MG   | 2     | 1947 | 1/1   | 0.86 | 0.21 | 50,50,50,50                 | 0     |
| 86  | OHX  | 4     | 232  | 7/7   | 0.86 | 0.21 | 93,93,93,93                 | 0     |
| 86  | OHX  | 4     | 233  | 7/7   | 0.86 | 0.17 | 121,121,121,121             | 0     |
| 86  | OHX  | 5     | 4241 | 7/7   | 0.86 | 0.28 | 81,81,81,81                 | 0     |
| 85  | MG   | 6     | 2038 | 1/1   | 0.86 | 0.37 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3839 | 1/1   | 0.86 | 0.09 | 30,30,30,30                 | 0     |
| 85  | MG   | 3     | 208  | 1/1   | 0.86 | 0.24 | 66,66,66,66                 | 0     |
| 85  | MG   | 1     | 3507 | 1/1   | 0.86 | 0.24 | 22,22,22,22                 | 0     |
| 85  | MG   | 6     | 1937 | 1/1   | 0.86 | 0.26 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3508 | 1/1   | 0.86 | 0.25 | 19,19,19,19                 | 0     |
| 85  | MG   | 5     | 3858 | 1/1   | 0.86 | 0.26 | 70,70,70,70                 | 0     |
| 86  | OHX  | 8     | 224  | 7/7   | 0.86 | 0.21 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3515 | 1/1   | 0.86 | 0.34 | 29,29,29,29                 | 0     |
| 85  | MG   | 4     | 201  | 1/1   | 0.86 | 0.32 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4073 | 7/7   | 0.86 | 0.23 | 94,94,94,94                 | 0     |
| 86  | OHX  | m0    | 302  | 7/7   | 0.86 | 0.24 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 4092 | 7/7   | 0.86 | 0.27 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2152 | 7/7   | 0.86 | 0.19 | 126,126,126,126             | 0     |
| 86  | OHX  | 6     | 2159 | 7/7   | 0.86 | 0.20 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 4096 | 7/7   | 0.86 | 0.16 | 123,123,123,123             | 0     |
| 86  | OHX  | 6     | 2169 | 7/7   | 0.86 | 0.18 | 124,124,124,124             | 0     |
| 86  | OHX  | 2     | 2137 | 7/7   | 0.87 | 0.21 | 104,104,104,104             | 0     |
| 86  | OHX  | 6     | 2198 | 7/7   | 0.87 | 0.20 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3808 | 1/1   | 0.87 | 0.12 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3635 | 1/1   | 0.87 | 0.33 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3436 | 1/1   | 0.87 | 0.20 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3663 | 1/1   | 0.87 | 0.10 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3685 | 1/1   | 0.87 | 0.15 | 45,45,45,45                 | 0     |
| 86  | OHX  | s8    | 303  | 7/7   | 0.87 | 0.18 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3502 | 1/1   | 0.87 | 0.28 | 35,35,35,35                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2152 | 7/7   | 0.87 | 0.15 | 145,145,145,145             | 0     |
| 86  | OHX  | d4    | 201  | 7/7   | 0.87 | 0.17 | 120,120,120,120             | 0     |
| 86  | OHX  | 2     | 2156 | 7/7   | 0.87 | 0.19 | 114,114,114,114             | 0     |
| 86  | OHX  | 5     | 4137 | 7/7   | 0.87 | 0.24 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 4138 | 7/7   | 0.87 | 0.18 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3834 | 1/1   | 0.87 | 0.09 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3465 | 1/1   | 0.87 | 0.21 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3428 | 1/1   | 0.87 | 0.19 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4147 | 7/7   | 0.87 | 0.21 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3467 | 1/1   | 0.87 | 0.20 | 31,31,31,31                 | 0     |
| 85  | MG   | 4     | 214  | 1/1   | 0.87 | 0.12 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 4155 | 7/7   | 0.87 | 0.18 | 111,111,111,111             | 0     |
| 86  | OHX  | 5     | 4157 | 7/7   | 0.87 | 0.24 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3854 | 1/1   | 0.87 | 0.10 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3746 | 1/1   | 0.87 | 0.16 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3689 | 1/1   | 0.87 | 0.07 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3841 | 1/1   | 0.87 | 0.28 | 37,37,37,37                 | 0     |
| 86  | OHX  | 5     | 4167 | 7/7   | 0.87 | 0.21 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3705 | 1/1   | 0.87 | 0.14 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4179 | 7/7   | 0.87 | 0.20 | 113,113,113,113             | 0     |
| 86  | OHX  | 5     | 4180 | 7/7   | 0.87 | 0.18 | 120,120,120,120             | 0     |
| 86  | OHX  | 2     | 2172 | 7/7   | 0.87 | 0.19 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4182 | 7/7   | 0.87 | 0.22 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4185 | 7/7   | 0.87 | 0.24 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4201 | 7/7   | 0.87 | 0.21 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 4188 | 7/7   | 0.87 | 0.18 | 111,111,111,111             | 0     |
| 85  | MG   | 1     | 3690 | 1/1   | 0.87 | 0.29 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3712 | 1/1   | 0.87 | 0.11 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3481 | 1/1   | 0.87 | 0.25 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3718 | 1/1   | 0.87 | 0.10 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3758 | 1/1   | 0.87 | 0.09 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3488 | 1/1   | 0.87 | 0.18 | 41,41,41,41                 | 0     |
| 86  | OHX  | S8    | 302  | 7/7   | 0.87 | 0.17 | 126,126,126,126             | 0     |
| 85  | MG   | 6     | 1964 | 1/1   | 0.87 | 0.25 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4213 | 7/7   | 0.87 | 0.16 | 128,128,128,128             | 0     |
| 85  | MG   | 6     | 2036 | 1/1   | 0.87 | 0.32 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 4208 | 7/7   | 0.87 | 0.20 | 110,110,110,110             | 0     |
| 86  | OHX  | 1     | 4085 | 7/7   | 0.87 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3649 | 1/1   | 0.87 | 0.11 | 19,19,19,19                 | 0     |
| 86  | OHX  | 1     | 4093 | 7/7   | 0.87 | 0.19 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3703 | 1/1   | 0.87 | 0.25 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 4099 | 7/7   | 0.87 | 0.17 | 115,115,115,115             | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86  | OHX  | 5     | 4216 | 7/7   | 0.87 | 0.20 | 113,113,113,113            | 0     |
| 86  | OHX  | 1     | 4111 | 7/7   | 0.87 | 0.21 | 110,110,110,110            | 0     |
| 85  | MG   | 1     | 3773 | 1/1   | 0.87 | 0.12 | 37,37,37,37                | 0     |
| 86  | OHX  | 1     | 4119 | 7/7   | 0.87 | 0.21 | 103,103,103,103            | 0     |
| 86  | OHX  | 1     | 4128 | 7/7   | 0.87 | 0.25 | 96,96,96,96                | 0     |
| 86  | OHX  | 5     | 4221 | 7/7   | 0.87 | 0.19 | 113,113,113,113            | 0     |
| 85  | MG   | 1     | 3429 | 1/1   | 0.87 | 0.20 | 36,36,36,36                | 0     |
| 85  | MG   | 5     | 3748 | 1/1   | 0.87 | 0.24 | 29,29,29,29                | 0     |
| 85  | MG   | 5     | 3542 | 1/1   | 0.87 | 0.28 | 53,53,53,53                | 0     |
| 85  | MG   | 1     | 3785 | 1/1   | 0.87 | 0.28 | 55,55,55,55                | 0     |
| 85  | MG   | 5     | 3564 | 1/1   | 0.87 | 0.31 | 38,38,38,38                | 0     |
| 85  | MG   | 1     | 3617 | 1/1   | 0.87 | 0.22 | 48,48,48,48                | 0     |
| 85  | MG   | 1     | 3420 | 1/1   | 0.87 | 0.44 | 57,57,57,57                | 0     |
| 85  | MG   | 1     | 3795 | 1/1   | 0.87 | 0.19 | 51,51,51,51                | 0     |
| 86  | OHX  | 6     | 2160 | 7/7   | 0.87 | 0.24 | 103,103,103,103            | 0     |
| 86  | OHX  | 6     | 2164 | 7/7   | 0.87 | 0.13 | 153,153,153,153            | 0     |
| 85  | MG   | 5     | 3580 | 1/1   | 0.87 | 0.31 | 36,36,36,36                | 0     |
| 85  | MG   | 5     | 3588 | 1/1   | 0.87 | 0.29 | 30,30,30,30                | 0     |
| 85  | MG   | 1     | 3414 | 1/1   | 0.87 | 0.18 | 28,28,28,28                | 0     |
| 86  | OHX  | 6     | 2173 | 7/7   | 0.87 | 0.20 | 116,116,116,116            | 0     |
| 85  | MG   | 1     | 3448 | 1/1   | 0.87 | 0.12 | 32,32,32,32                | 0     |
| 85  | MG   | 5     | 3403 | 1/1   | 0.87 | 0.37 | 53,53,53,53                | 0     |
| 86  | OHX  | 6     | 2177 | 7/7   | 0.87 | 0.24 | 97,97,97,97                | 0     |
| 86  | OHX  | 5     | 4242 | 7/7   | 0.87 | 0.17 | 124,124,124,124            | 0     |
| 85  | MG   | 5     | 3409 | 1/1   | 0.87 | 0.23 | 39,39,39,39                | 0     |
| 86  | OHX  | 1     | 4150 | 7/7   | 0.87 | 0.19 | 111,111,111,111            | 0     |
| 86  | OHX  | 6     | 2180 | 7/7   | 0.87 | 0.22 | 106,106,106,106            | 0     |
| 85  | MG   | 1     | 3718 | 1/1   | 0.87 | 0.18 | 33,33,33,33                | 0     |
| 85  | MG   | 5     | 3635 | 1/1   | 0.87 | 0.23 | 39,39,39,39                | 0     |
| 86  | OHX  | 5     | 4250 | 7/7   | 0.87 | 0.17 | 128,128,128,128            | 0     |
| 86  | OHX  | 1     | 4163 | 7/7   | 0.87 | 0.18 | 118,118,118,118            | 0     |
| 86  | OHX  | 1     | 4165 | 7/7   | 0.87 | 0.17 | 123,123,123,123            | 0     |
| 85  | MG   | n8    | 202  | 1/1   | 0.87 | 0.11 | 19,19,19,19                | 0     |
| 85  | MG   | 6     | 1918 | 1/1   | 0.87 | 0.43 | 57,57,57,57                | 0     |
| 86  | OHX  | 14    | 402  | 7/7   | 0.87 | 0.19 | 103,103,103,103            | 0     |
| 85  | MG   | 6     | 1996 | 1/1   | 0.87 | 0.27 | 62,62,62,62                | 0     |
| 85  | MG   | 5     | 3643 | 1/1   | 0.87 | 0.13 | 37,37,37,37                | 0     |
| 86  | OHX  | 2     | 2094 | 7/7   | 0.87 | 0.16 | 119,119,119,119            | 0     |
| 85  | MG   | 2     | 1992 | 1/1   | 0.87 | 0.10 | 50,50,50,50                | 0     |
| 85  | MG   | 2     | 1970 | 1/1   | 0.87 | 0.25 | 60,60,60,60                | 0     |
| 86  | OHX  | m7    | 206  | 7/7   | 0.87 | 0.23 | 99,99,99,99                | 0     |
| 85  | MG   | 5     | 3653 | 1/1   | 0.87 | 0.15 | 46,46,46,46                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2136 | 7/7   | 0.87 | 0.19 | 107,107,107,107             | 0     |
| 86  | OHX  | 1     | 4176 | 7/7   | 0.87 | 0.15 | 133,133,133,133             | 0     |
| 85  | MG   | 1     | 3582 | 1/1   | 0.88 | 0.25 | 30,30,30,30                 | 0     |
| 85  | MG   | 6     | 2028 | 1/1   | 0.88 | 0.38 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 4155 | 7/7   | 0.88 | 0.18 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3526 | 1/1   | 0.88 | 0.31 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3521 | 1/1   | 0.88 | 0.32 | 60,60,60,60                 | 0     |
| 85  | MG   | 5     | 3536 | 1/1   | 0.88 | 0.19 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3781 | 1/1   | 0.88 | 0.09 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3547 | 1/1   | 0.88 | 0.30 | 32,32,32,32                 | 0     |
| 85  | MG   | 6     | 1925 | 1/1   | 0.88 | 0.33 | 34,34,34,34                 | 0     |
| 85  | MG   | 6     | 1928 | 1/1   | 0.88 | 0.34 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3591 | 1/1   | 0.88 | 0.28 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3567 | 1/1   | 0.88 | 0.20 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4108 | 7/7   | 0.88 | 0.23 | 95,95,95,95                 | 0     |
| 85  | MG   | 1     | 3641 | 1/1   | 0.88 | 0.11 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4131 | 7/7   | 0.88 | 0.13 | 147,147,147,147             | 0     |
| 86  | OHX  | 5     | 4136 | 7/7   | 0.88 | 0.19 | 103,103,103,103             | 0     |
| 86  | OHX  | 2     | 2108 | 7/7   | 0.88 | 0.18 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3457 | 1/1   | 0.88 | 0.19 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3459 | 1/1   | 0.88 | 0.29 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 4140 | 7/7   | 0.88 | 0.19 | 101,101,101,101             | 0     |
| 85  | MG   | 3     | 213  | 1/1   | 0.88 | 0.38 | 49,49,49,49                 | 0     |
| 86  | OHX  | 2     | 2134 | 7/7   | 0.88 | 0.14 | 127,127,127,127             | 0     |
| 86  | OHX  | 2     | 2135 | 7/7   | 0.88 | 0.19 | 108,108,108,108             | 0     |
| 86  | OHX  | 5     | 4148 | 7/7   | 0.88 | 0.17 | 119,119,119,119             | 0     |
| 85  | MG   | 5     | 3590 | 1/1   | 0.88 | 0.24 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3538 | 1/1   | 0.88 | 0.15 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3608 | 1/1   | 0.88 | 0.19 | 50,50,50,50                 | 0     |
| 85  | MG   | 6     | 1951 | 1/1   | 0.88 | 0.36 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 4158 | 7/7   | 0.88 | 0.22 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3805 | 1/1   | 0.88 | 0.18 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3806 | 1/1   | 0.88 | 0.17 | 48,48,48,48                 | 0     |
| 85  | MG   | c1    | 201  | 1/1   | 0.88 | 0.14 | 41,41,41,41                 | 0     |
| 86  | OHX  | 2     | 2148 | 7/7   | 0.88 | 0.14 | 142,142,142,142             | 0     |
| 86  | OHX  | 2     | 2149 | 7/7   | 0.88 | 0.22 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4169 | 7/7   | 0.88 | 0.16 | 130,130,130,130             | 0     |
| 85  | MG   | 2     | 1966 | 1/1   | 0.88 | 0.24 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 4176 | 7/7   | 0.88 | 0.26 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2151 | 7/7   | 0.88 | 0.17 | 134,134,134,134             | 0     |
| 85  | MG   | 4     | 212  | 1/1   | 0.88 | 0.09 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4194 | 7/7   | 0.88 | 0.18 | 114,114,114,114             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2153 | 7/7   | 0.88 | 0.17 | 118,118,118,118             | 0     |
| 86  | OHX  | 2     | 2154 | 7/7   | 0.88 | 0.17 | 131,131,131,131             | 0     |
| 86  | OHX  | 2     | 2155 | 7/7   | 0.88 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3641 | 1/1   | 0.88 | 0.25 | 47,47,47,47                 | 0     |
| 85  | MG   | 2     | 2021 | 1/1   | 0.88 | 0.45 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4191 | 7/7   | 0.88 | 0.21 | 97,97,97,97                 | 0     |
| 85  | MG   | 4     | 215  | 1/1   | 0.88 | 0.16 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3410 | 1/1   | 0.88 | 0.24 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3828 | 1/1   | 0.88 | 0.24 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3832 | 1/1   | 0.88 | 0.08 | 37,37,37,37                 | 0     |
| 85  | MG   | 6     | 1969 | 1/1   | 0.88 | 0.14 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3724 | 1/1   | 0.88 | 0.10 | 43,43,43,43                 | 0     |
| 85  | MG   | 2     | 1912 | 1/1   | 0.88 | 0.23 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3670 | 1/1   | 0.88 | 0.26 | 65,65,65,65                 | 0     |
| 86  | OHX  | 2     | 2167 | 7/7   | 0.88 | 0.15 | 132,132,132,132             | 0     |
| 86  | OHX  | 5     | 4207 | 7/7   | 0.88 | 0.25 | 89,89,89,89                 | 0     |
| 85  | MG   | 5     | 3851 | 1/1   | 0.88 | 0.23 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3412 | 1/1   | 0.88 | 0.33 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3431 | 1/1   | 0.88 | 0.25 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2175 | 7/7   | 0.88 | 0.15 | 128,128,128,128             | 0     |
| 86  | OHX  | 4     | 231  | 7/7   | 0.88 | 0.18 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3676 | 1/1   | 0.88 | 0.22 | 81,81,81,81                 | 0     |
| 86  | OHX  | 2     | 2177 | 7/7   | 0.88 | 0.21 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3432 | 1/1   | 0.88 | 0.28 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3674 | 1/1   | 0.88 | 0.36 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3861 | 1/1   | 0.88 | 0.09 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3863 | 1/1   | 0.88 | 0.25 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3437 | 1/1   | 0.88 | 0.20 | 45,45,45,45                 | 0     |
| 85  | MG   | L8    | 301  | 1/1   | 0.88 | 0.33 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3693 | 1/1   | 0.88 | 0.22 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3737 | 1/1   | 0.88 | 0.26 | 54,54,54,54                 | 0     |
| 85  | MG   | 2     | 2011 | 1/1   | 0.88 | 0.38 | 59,59,59,59                 | 0     |
| 86  | OHX  | 6     | 2135 | 7/7   | 0.88 | 0.16 | 116,116,116,116             | 0     |
| 85  | MG   | 6     | 1991 | 1/1   | 0.88 | 0.26 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 4228 | 7/7   | 0.88 | 0.15 | 141,141,141,141             | 0     |
| 85  | MG   | 1     | 3683 | 1/1   | 0.88 | 0.12 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3625 | 1/1   | 0.88 | 0.17 | 27,27,27,27                 | 0     |
| 86  | OHX  | 5     | 4231 | 7/7   | 0.88 | 0.14 | 137,137,137,137             | 0     |
| 86  | OHX  | 6     | 2156 | 7/7   | 0.88 | 0.16 | 119,119,119,119             | 0     |
| 85  | MG   | 5     | 3885 | 1/1   | 0.88 | 0.30 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 4115 | 7/7   | 0.88 | 0.20 | 106,106,106,106             | 0     |
| 85  | MG   | 2     | 1993 | 1/1   | 0.88 | 0.12 | 46,46,46,46                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4117 | 7/7   | 0.88 | 0.15 | 136,136,136,136             | 0     |
| 86  | OHX  | 6     | 2167 | 7/7   | 0.88 | 0.15 | 140,140,140,140             | 0     |
| 86  | OHX  | 6     | 2168 | 7/7   | 0.88 | 0.24 | 97,97,97,97                 | 0     |
| 85  | MG   | 2     | 1917 | 1/1   | 0.88 | 0.32 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4122 | 7/7   | 0.88 | 0.20 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4123 | 7/7   | 0.88 | 0.22 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4124 | 7/7   | 0.88 | 0.21 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 4126 | 7/7   | 0.88 | 0.20 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 2001 | 1/1   | 0.88 | 0.15 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 4129 | 7/7   | 0.88 | 0.17 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3889 | 1/1   | 0.88 | 0.10 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3721 | 1/1   | 0.88 | 0.28 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3722 | 1/1   | 0.88 | 0.10 | 39,39,39,39                 | 0     |
| 86  | OHX  | 6     | 2182 | 7/7   | 0.88 | 0.19 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3688 | 1/1   | 0.88 | 0.13 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3761 | 1/1   | 0.88 | 0.11 | 42,42,42,42                 | 0     |
| 86  | OHX  | 8     | 228  | 7/7   | 0.88 | 0.20 | 101,101,101,101             | 0     |
| 86  | OHX  | 8     | 229  | 7/7   | 0.88 | 0.20 | 108,108,108,108             | 0     |
| 86  | OHX  | l3    | 404  | 7/7   | 0.88 | 0.19 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3762 | 1/1   | 0.88 | 0.09 | 24,24,24,24                 | 0     |
| 86  | OHX  | 1     | 4137 | 7/7   | 0.88 | 0.20 | 89,89,89,89                 | 0     |
| 85  | MG   | 1     | 3862 | 1/1   | 0.88 | 0.11 | 41,41,41,41                 | 0     |
| 85  | MG   | 7     | 209  | 1/1   | 0.88 | 0.32 | 35,35,35,35                 | 0     |
| 85  | MG   | 7     | 211  | 1/1   | 0.88 | 0.17 | 46,46,46,46                 | 0     |
| 85  | MG   | 7     | 212  | 1/1   | 0.88 | 0.16 | 64,64,64,64                 | 0     |
| 85  | MG   | 1     | 3763 | 1/1   | 0.88 | 0.11 | 38,38,38,38                 | 0     |
| 85  | MG   | 6     | 2018 | 1/1   | 0.88 | 0.09 | 44,44,44,44                 | 0     |
| 85  | MG   | 2     | 1974 | 1/1   | 0.88 | 0.25 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3745 | 1/1   | 0.88 | 0.22 | 33,33,33,33                 | 0     |
| 88  | 3H3  | 1     | 4216 | 33/33 | 0.88 | 0.14 | 26,26,26,26                 | 0     |
| 86  | OHX  | 1     | 4149 | 7/7   | 0.89 | 0.18 | 105,105,105,105             | 0     |
| 85  | MG   | 2     | 1995 | 1/1   | 0.89 | 0.45 | 75,75,75,75                 | 0     |
| 85  | MG   | m1    | 201  | 1/1   | 0.89 | 0.25 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3585 | 1/1   | 0.89 | 0.35 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 4160 | 7/7   | 0.89 | 0.18 | 114,114,114,114             | 0     |
| 85  | MG   | n6    | 202  | 1/1   | 0.89 | 0.13 | 34,34,34,34                 | 0     |
| 85  | MG   | 2     | 1920 | 1/1   | 0.89 | 0.14 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 2022 | 1/1   | 0.89 | 0.14 | 71,71,71,71                 | 0     |
| 85  | MG   | 5     | 3491 | 1/1   | 0.89 | 0.11 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4096 | 7/7   | 0.89 | 0.17 | 115,115,115,115             | 0     |
| 86  | OHX  | 5     | 4098 | 7/7   | 0.89 | 0.17 | 114,114,114,114             | 0     |
| 86  | OHX  | 5     | 4101 | 7/7   | 0.89 | 0.16 | 121,121,121,121             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 2025 | 1/1   | 0.89 | 0.17 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3784 | 1/1   | 0.89 | 0.12 | 29,29,29,29                 | 0     |
| 86  | OHX  | 5     | 4123 | 7/7   | 0.89 | 0.15 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3498 | 1/1   | 0.89 | 0.25 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3516 | 1/1   | 0.89 | 0.26 | 28,28,28,28                 | 0     |
| 85  | MG   | 2     | 2014 | 1/1   | 0.89 | 0.40 | 61,61,61,61                 | 0     |
| 85  | MG   | 5     | 3516 | 1/1   | 0.89 | 0.29 | 20,20,20,20                 | 0     |
| 85  | MG   | 5     | 3517 | 1/1   | 0.89 | 0.22 | 18,18,18,18                 | 0     |
| 86  | OHX  | 2     | 2128 | 7/7   | 0.89 | 0.19 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4142 | 7/7   | 0.89 | 0.21 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3788 | 1/1   | 0.89 | 0.23 | 48,48,48,48                 | 0     |
| 85  | MG   | 2     | 2015 | 1/1   | 0.89 | 0.35 | 59,59,59,59                 | 0     |
| 85  | MG   | 6     | 2032 | 1/1   | 0.89 | 0.22 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3719 | 1/1   | 0.89 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 2     | 1985 | 1/1   | 0.89 | 0.09 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3548 | 1/1   | 0.89 | 0.32 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4154 | 7/7   | 0.89 | 0.19 | 106,106,106,106             | 0     |
| 85  | MG   | 2     | 1998 | 1/1   | 0.89 | 0.21 | 60,60,60,60                 | 0     |
| 85  | MG   | 5     | 3552 | 1/1   | 0.89 | 0.24 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3554 | 1/1   | 0.89 | 0.20 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4186 | 7/7   | 0.89 | 0.17 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3556 | 1/1   | 0.89 | 0.19 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3727 | 1/1   | 0.89 | 0.15 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3609 | 1/1   | 0.89 | 0.32 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 4166 | 7/7   | 0.89 | 0.16 | 120,120,120,120             | 0     |
| 85  | MG   | 1     | 3455 | 1/1   | 0.89 | 0.24 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3802 | 1/1   | 0.89 | 0.11 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4173 | 7/7   | 0.89 | 0.20 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3671 | 1/1   | 0.89 | 0.18 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3570 | 1/1   | 0.89 | 0.28 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4177 | 7/7   | 0.89 | 0.19 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3575 | 1/1   | 0.89 | 0.30 | 33,33,33,33                 | 0     |
| 85  | MG   | 6     | 1957 | 1/1   | 0.89 | 0.44 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 2044 | 1/1   | 0.89 | 0.36 | 44,44,44,44                 | 0     |
| 86  | OHX  | 2     | 2158 | 7/7   | 0.89 | 0.21 | 93,93,93,93                 | 0     |
| 85  | MG   | 5     | 3586 | 1/1   | 0.89 | 0.27 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3587 | 1/1   | 0.89 | 0.27 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3544 | 1/1   | 0.89 | 0.21 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4189 | 7/7   | 0.89 | 0.19 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3825 | 1/1   | 0.89 | 0.12 | 31,31,31,31                 | 0     |
| 85  | MG   | 6     | 1959 | 1/1   | 0.89 | 0.40 | 52,52,52,52                 | 0     |
| 85  | MG   | s6    | 301  | 1/1   | 0.89 | 0.39 | 59,59,59,59                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3545 | 1/1   | 0.89 | 0.24 | 37,37,37,37                 | 0     |
| 85  | MG   | 2     | 1927 | 1/1   | 0.89 | 0.35 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3617 | 1/1   | 0.89 | 0.09 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 4208 | 7/7   | 0.89 | 0.22 | 100,100,100,100             | 0     |
| 86  | OHX  | 1     | 4209 | 7/7   | 0.89 | 0.20 | 104,104,104,104             | 0     |
| 86  | OHX  | 2     | 2168 | 7/7   | 0.89 | 0.14 | 135,135,135,135             | 0     |
| 85  | MG   | 5     | 3844 | 1/1   | 0.89 | 0.12 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3620 | 1/1   | 0.89 | 0.07 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 3847 | 1/1   | 0.89 | 0.24 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3739 | 1/1   | 0.89 | 0.25 | 53,53,53,53                 | 0     |
| 85  | MG   | d6    | 102  | 1/1   | 0.89 | 0.16 | 47,47,47,47                 | 0     |
| 86  | OHX  | 3     | 225  | 7/7   | 0.89 | 0.22 | 103,103,103,103             | 0     |
| 86  | OHX  | 3     | 226  | 7/7   | 0.89 | 0.19 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3740 | 1/1   | 0.89 | 0.14 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 4213 | 7/7   | 0.89 | 0.11 | 166,166,166,166             | 0     |
| 85  | MG   | 2     | 1940 | 1/1   | 0.89 | 0.26 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3407 | 1/1   | 0.89 | 0.15 | 32,32,32,32                 | 0     |
| 85  | MG   | 2     | 1932 | 1/1   | 0.89 | 0.38 | 48,48,48,48                 | 0     |
| 85  | MG   | 2     | 1942 | 1/1   | 0.89 | 0.25 | 63,63,63,63                 | 0     |
| 85  | MG   | 5     | 3413 | 1/1   | 0.89 | 0.20 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4020 | 7/7   | 0.89 | 0.12 | 127,127,127,127             | 0     |
| 86  | OHX  | L4    | 404  | 7/7   | 0.89 | 0.19 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4024 | 7/7   | 0.89 | 0.20 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4031 | 7/7   | 0.89 | 0.22 | 88,88,88,88                 | 0     |
| 85  | MG   | M1    | 201  | 1/1   | 0.89 | 0.22 | 61,61,61,61                 | 0     |
| 85  | MG   | 2     | 1943 | 1/1   | 0.89 | 0.26 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 4084 | 7/7   | 0.89 | 0.22 | 89,89,89,89                 | 0     |
| 86  | OHX  | 6     | 2105 | 7/7   | 0.89 | 0.19 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3868 | 1/1   | 0.89 | 0.43 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3871 | 1/1   | 0.89 | 0.44 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3629 | 1/1   | 0.89 | 0.12 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3656 | 1/1   | 0.89 | 0.08 | 35,35,35,35                 | 0     |
| 86  | OHX  | 1     | 4098 | 7/7   | 0.89 | 0.19 | 103,103,103,103             | 0     |
| 85  | MG   | 6     | 1979 | 1/1   | 0.89 | 0.31 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4103 | 7/7   | 0.89 | 0.20 | 98,98,98,98                 | 0     |
| 86  | OHX  | 1     | 4104 | 7/7   | 0.89 | 0.16 | 119,119,119,119             | 0     |
| 85  | MG   | M5    | 301  | 1/1   | 0.89 | 0.11 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4113 | 7/7   | 0.89 | 0.19 | 106,106,106,106             | 0     |
| 85  | MG   | 5     | 3666 | 1/1   | 0.89 | 0.09 | 21,21,21,21                 | 0     |
| 85  | MG   | 5     | 3430 | 1/1   | 0.89 | 0.15 | 27,27,27,27                 | 0     |
| 85  | MG   | M5    | 302  | 1/1   | 0.89 | 0.11 | 46,46,46,46                 | 0     |
| 85  | MG   | M7    | 202  | 1/1   | 0.89 | 0.21 | 26,26,26,26                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4243 | 7/7   | 0.89 | 0.19 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3678 | 1/1   | 0.89 | 0.12 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3433 | 1/1   | 0.89 | 0.28 | 64,64,64,64                 | 0     |
| 86  | OHX  | 6     | 2176 | 7/7   | 0.89 | 0.23 | 87,87,87,87                 | 0     |
| 85  | MG   | 2     | 1933 | 1/1   | 0.89 | 0.32 | 57,57,57,57                 | 0     |
| 85  | MG   | 6     | 1990 | 1/1   | 0.89 | 0.29 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4249 | 7/7   | 0.89 | 0.18 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3441 | 1/1   | 0.89 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3563 | 1/1   | 0.89 | 0.22 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3451 | 1/1   | 0.89 | 0.10 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4131 | 7/7   | 0.89 | 0.22 | 102,102,102,102             | 0     |
| 85  | MG   | 1     | 3856 | 1/1   | 0.89 | 0.10 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3460 | 1/1   | 0.89 | 0.08 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3464 | 1/1   | 0.89 | 0.08 | 30,30,30,30                 | 0     |
| 85  | MG   | Q2    | 502  | 1/1   | 0.89 | 0.25 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3857 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3468 | 1/1   | 0.89 | 0.21 | 37,37,37,37                 | 0     |
| 86  | OHX  | l5    | 304  | 7/7   | 0.89 | 0.15 | 116,116,116,116             | 0     |
| 85  | MG   | 1     | 3766 | 1/1   | 0.89 | 0.20 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3473 | 1/1   | 0.89 | 0.23 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3565 | 1/1   | 0.89 | 0.12 | 27,27,27,27                 | 0     |
| 86  | OHX  | 1     | 4143 | 7/7   | 0.89 | 0.19 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3469 | 1/1   | 0.89 | 0.31 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3770 | 1/1   | 0.89 | 0.19 | 75,75,75,75                 | 0     |
| 85  | MG   | 6     | 1916 | 1/1   | 0.89 | 0.39 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3734 | 1/1   | 0.89 | 0.32 | 58,58,58,58                 | 0     |
| 85  | MG   | l2    | 301  | 1/1   | 0.89 | 0.24 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4140 | 7/7   | 0.90 | 0.21 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3698 | 1/1   | 0.90 | 0.33 | 62,62,62,62                 | 0     |
| 86  | OHX  | 6     | 2197 | 7/7   | 0.90 | 0.18 | 113,113,113,113             | 0     |
| 85  | MG   | O3    | 201  | 1/1   | 0.90 | 0.07 | 28,28,28,28                 | 0     |
| 85  | MG   | 6     | 2008 | 1/1   | 0.90 | 0.12 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3720 | 1/1   | 0.90 | 0.09 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3587 | 1/1   | 0.90 | 0.30 | 26,26,26,26                 | 0     |
| 85  | MG   | 6     | 1902 | 1/1   | 0.90 | 0.20 | 47,47,47,47                 | 0     |
| 85  | MG   | l5    | 302  | 1/1   | 0.90 | 0.28 | 54,54,54,54                 | 0     |
| 85  | MG   | 6     | 2017 | 1/1   | 0.90 | 0.17 | 58,58,58,58                 | 0     |
| 85  | MG   | l7    | 301  | 1/1   | 0.90 | 0.22 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3526 | 1/1   | 0.90 | 0.24 | 21,21,21,21                 | 0     |
| 86  | OHX  | c5    | 201  | 7/7   | 0.90 | 0.14 | 127,127,127,127             | 0     |
| 86  | OHX  | 1     | 4151 | 7/7   | 0.90 | 0.16 | 113,113,113,113             | 0     |
| 86  | OHX  | 5     | 4017 | 7/7   | 0.90 | 0.15 | 128,128,128,128             | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4027 | 7/7   | 0.90 | 0.17 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 4062 | 7/7   | 0.90 | 0.18 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4063 | 7/7   | 0.90 | 0.17 | 106,106,106,106             | 0     |
| 85  | MG   | m1    | 202  | 1/1   | 0.90 | 0.16 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 4154 | 7/7   | 0.90 | 0.19 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3495 | 1/1   | 0.90 | 0.17 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4105 | 7/7   | 0.90 | 0.23 | 87,87,87,87                 | 0     |
| 85  | MG   | 6     | 2020 | 1/1   | 0.90 | 0.12 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 4161 | 7/7   | 0.90 | 0.18 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4122 | 7/7   | 0.90 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 2     | 1989 | 1/1   | 0.90 | 0.29 | 65,65,65,65                 | 0     |
| 85  | MG   | 1     | 3483 | 1/1   | 0.90 | 0.22 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4164 | 7/7   | 0.90 | 0.19 | 108,108,108,108             | 0     |
| 85  | MG   | n8    | 203  | 1/1   | 0.90 | 0.24 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3739 | 1/1   | 0.90 | 0.16 | 31,31,31,31                 | 0     |
| 85  | MG   | 2     | 1901 | 1/1   | 0.90 | 0.45 | 57,57,57,57                 | 0     |
| 85  | MG   | 5     | 3514 | 1/1   | 0.90 | 0.19 | 22,22,22,22                 | 0     |
| 85  | MG   | 1     | 3650 | 1/1   | 0.90 | 0.10 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1914 | 1/1   | 0.90 | 0.25 | 29,29,29,29                 | 0     |
| 86  | OHX  | 2     | 2112 | 7/7   | 0.90 | 0.16 | 130,130,130,130             | 0     |
| 85  | MG   | 1     | 3774 | 1/1   | 0.90 | 0.23 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3780 | 1/1   | 0.90 | 0.20 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 4149 | 7/7   | 0.90 | 0.23 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4150 | 7/7   | 0.90 | 0.17 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3531 | 1/1   | 0.90 | 0.24 | 31,31,31,31                 | 0     |
| 85  | MG   | 6     | 1917 | 1/1   | 0.90 | 0.29 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3763 | 1/1   | 0.90 | 0.15 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3540 | 1/1   | 0.90 | 0.29 | 28,28,28,28                 | 0     |
| 86  | OHX  | 5     | 4156 | 7/7   | 0.90 | 0.18 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3598 | 1/1   | 0.90 | 0.29 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3544 | 1/1   | 0.90 | 0.32 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4181 | 7/7   | 0.90 | 0.08 | 192,192,192,192             | 0     |
| 85  | MG   | 5     | 3545 | 1/1   | 0.90 | 0.24 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2139 | 7/7   | 0.90 | 0.16 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3546 | 1/1   | 0.90 | 0.22 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3771 | 1/1   | 0.90 | 0.15 | 55,55,55,55                 | 0     |
| 86  | OHX  | 2     | 2143 | 7/7   | 0.90 | 0.17 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3486 | 1/1   | 0.90 | 0.09 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4172 | 7/7   | 0.90 | 0.21 | 102,102,102,102             | 0     |
| 85  | MG   | 1     | 4219 | 1/1   | 0.90 | 0.19 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3778 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 4175 | 7/7   | 0.90 | 0.19 | 105,105,105,105             | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 4221 | 1/1   | 0.90 | 0.10 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 2037 | 1/1   | 0.90 | 0.29 | 52,52,52,52                 | 0     |
| 85  | MG   | 2     | 1911 | 1/1   | 0.90 | 0.34 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3783 | 1/1   | 0.90 | 0.11 | 50,50,50,50                 | 0     |
| 85  | MG   | 6     | 1926 | 1/1   | 0.90 | 0.23 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3436 | 1/1   | 0.90 | 0.16 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4183 | 7/7   | 0.90 | 0.20 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 4184 | 7/7   | 0.90 | 0.21 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3722 | 1/1   | 0.90 | 0.09 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3492 | 1/1   | 0.90 | 0.15 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3613 | 1/1   | 0.90 | 0.27 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 1935 | 1/1   | 0.90 | 0.29 | 46,46,46,46                 | 0     |
| 85  | MG   | 6     | 2046 | 1/1   | 0.90 | 0.47 | 66,66,66,66                 | 0     |
| 85  | MG   | 5     | 3576 | 1/1   | 0.90 | 0.35 | 36,36,36,36                 | 0     |
| 85  | MG   | 3     | 211  | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 85  | MG   | 1     | 3668 | 1/1   | 0.90 | 0.09 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3799 | 1/1   | 0.90 | 0.28 | 21,21,21,21                 | 0     |
| 85  | MG   | 2     | 2182 | 1/1   | 0.90 | 0.18 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3444 | 1/1   | 0.90 | 0.29 | 49,49,49,49                 | 0     |
| 85  | MG   | c8    | 202  | 1/1   | 0.90 | 0.31 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3593 | 1/1   | 0.90 | 0.36 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3596 | 1/1   | 0.90 | 0.27 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3445 | 1/1   | 0.90 | 0.20 | 39,39,39,39                 | 0     |
| 85  | MG   | 6     | 1955 | 1/1   | 0.90 | 0.32 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3604 | 1/1   | 0.90 | 0.18 | 33,33,33,33                 | 0     |
| 86  | OHX  | 2     | 2174 | 7/7   | 0.90 | 0.17 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3619 | 1/1   | 0.90 | 0.27 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3616 | 1/1   | 0.90 | 0.14 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3845 | 1/1   | 0.90 | 0.10 | 44,44,44,44                 | 0     |
| 85  | MG   | 4     | 210  | 1/1   | 0.90 | 0.12 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3618 | 1/1   | 0.90 | 0.18 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3408 | 1/1   | 0.90 | 0.27 | 27,27,27,27                 | 0     |
| 85  | MG   | 6     | 1960 | 1/1   | 0.90 | 0.31 | 38,38,38,38                 | 0     |
| 85  | MG   | 2     | 2000 | 1/1   | 0.90 | 0.25 | 53,53,53,53                 | 0     |
| 86  | OHX  | C3    | 202  | 7/7   | 0.90 | 0.15 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3631 | 1/1   | 0.90 | 0.07 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3450 | 1/1   | 0.90 | 0.27 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3857 | 1/1   | 0.90 | 0.07 | 37,37,37,37                 | 0     |
| 86  | OHX  | 1     | 4065 | 7/7   | 0.90 | 0.16 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3514 | 1/1   | 0.90 | 0.21 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4067 | 7/7   | 0.90 | 0.21 | 100,100,100,100             | 0     |
| 86  | OHX  | 1     | 4071 | 7/7   | 0.90 | 0.20 | 99,99,99,99                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3750 | 1/1   | 0.90 | 0.09 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3862 | 1/1   | 0.90 | 0.09 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3825 | 1/1   | 0.90 | 0.15 | 31,31,31,31                 | 0     |
| 86  | OHX  | 6     | 2144 | 7/7   | 0.90 | 0.17 | 105,105,105,105             | 0     |
| 86  | OHX  | 1     | 4086 | 7/7   | 0.90 | 0.19 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 4091 | 7/7   | 0.90 | 0.20 | 98,98,98,98                 | 0     |
| 86  | OHX  | 6     | 2153 | 7/7   | 0.90 | 0.16 | 118,118,118,118             | 0     |
| 86  | OHX  | 6     | 2154 | 7/7   | 0.90 | 0.13 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3642 | 1/1   | 0.90 | 0.08 | 27,27,27,27                 | 0     |
| 86  | OHX  | 6     | 2158 | 7/7   | 0.90 | 0.16 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3826 | 1/1   | 0.90 | 0.25 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3627 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 86  | OHX  | 6     | 2163 | 7/7   | 0.90 | 0.19 | 106,106,106,106             | 0     |
| 85  | MG   | 6     | 1971 | 1/1   | 0.90 | 0.28 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3831 | 1/1   | 0.90 | 0.08 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4101 | 7/7   | 0.90 | 0.16 | 122,122,122,122             | 0     |
| 85  | MG   | 6     | 1973 | 1/1   | 0.90 | 0.14 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3435 | 1/1   | 0.90 | 0.07 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4106 | 7/7   | 0.90 | 0.17 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2172 | 7/7   | 0.90 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3658 | 1/1   | 0.90 | 0.08 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3453 | 1/1   | 0.90 | 0.21 | 37,37,37,37                 | 0     |
| 85  | MG   | L6    | 201  | 1/1   | 0.90 | 0.13 | 35,35,35,35                 | 0     |
| 85  | MG   | L7    | 301  | 1/1   | 0.90 | 0.16 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3425 | 1/1   | 0.90 | 0.13 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3837 | 1/1   | 0.90 | 0.10 | 30,30,30,30                 | 0     |
| 85  | MG   | M3    | 201  | 1/1   | 0.90 | 0.14 | 37,37,37,37                 | 0     |
| 86  | OHX  | 8     | 227  | 7/7   | 0.90 | 0.20 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3757 | 1/1   | 0.90 | 0.17 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1988 | 1/1   | 0.90 | 0.05 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4125 | 7/7   | 0.90 | 0.24 | 85,85,85,85                 | 0     |
| 85  | MG   | 5     | 3681 | 1/1   | 0.90 | 0.08 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3519 | 1/1   | 0.90 | 0.28 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3843 | 1/1   | 0.90 | 0.28 | 46,46,46,46                 | 0     |
| 85  | MG   | 2     | 1988 | 1/1   | 0.90 | 0.30 | 62,62,62,62                 | 0     |
| 86  | OHX  | 19    | 600  | 7/7   | 0.90 | 0.19 | 105,105,105,105             | 0     |
| 85  | MG   | 7     | 202  | 1/1   | 0.90 | 0.20 | 27,27,27,27                 | 0     |
| 85  | MG   | M7    | 201  | 1/1   | 0.90 | 0.43 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3471 | 1/1   | 0.90 | 0.08 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3698 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3847 | 1/1   | 0.90 | 0.29 | 49,49,49,49                 | 0     |
| 86  | OHX  | o4    | 203  | 7/7   | 0.90 | 0.20 | 104,104,104,104             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3849 | 1/1   | 0.90 | 0.19 | 33,33,33,33                 | 0     |
| 85  | MG   | N3    | 203  | 1/1   | 0.90 | 0.22 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3851 | 1/1   | 0.90 | 0.28 | 50,50,50,50                 | 0     |
| 85  | MG   | 2     | 1938 | 1/1   | 0.91 | 0.33 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3729 | 1/1   | 0.91 | 0.33 | 61,61,61,61                 | 0     |
| 85  | MG   | 2     | 2009 | 1/1   | 0.91 | 0.32 | 46,46,46,46                 | 0     |
| 85  | MG   | M6    | 201  | 1/1   | 0.91 | 0.08 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3733 | 1/1   | 0.91 | 0.15 | 32,32,32,32                 | 0     |
| 85  | MG   | d2    | 201  | 1/1   | 0.91 | 0.26 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3735 | 1/1   | 0.91 | 0.08 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3638 | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3522 | 1/1   | 0.91 | 0.31 | 27,27,27,27                 | 0     |
| 85  | MG   | M9    | 201  | 1/1   | 0.91 | 0.25 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 1974 | 1/1   | 0.91 | 0.17 | 45,45,45,45                 | 0     |
| 85  | MG   | m7    | 203  | 1/1   | 0.91 | 0.17 | 26,26,26,26                 | 0     |
| 85  | MG   | m7    | 205  | 1/1   | 0.91 | 0.07 | 26,26,26,26                 | 0     |
| 85  | MG   | 2     | 1956 | 1/1   | 0.91 | 0.20 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3860 | 1/1   | 0.91 | 0.28 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3527 | 1/1   | 0.91 | 0.31 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3416 | 1/1   | 0.91 | 0.21 | 21,21,21,21                 | 0     |
| 86  | OHX  | 5     | 3995 | 7/7   | 0.91 | 0.15 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3753 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3417 | 1/1   | 0.91 | 0.10 | 21,21,21,21                 | 0     |
| 86  | OHX  | 5     | 4037 | 7/7   | 0.91 | 0.18 | 94,94,94,94                 | 0     |
| 85  | MG   | o4    | 201  | 1/1   | 0.91 | 0.18 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3569 | 1/1   | 0.91 | 0.25 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 4089 | 7/7   | 0.91 | 0.25 | 84,84,84,84                 | 0     |
| 86  | OHX  | 1     | 4153 | 7/7   | 0.91 | 0.18 | 92,92,92,92                 | 0     |
| 85  | MG   | 1     | 3646 | 1/1   | 0.91 | 0.18 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4099 | 7/7   | 0.91 | 0.19 | 94,94,94,94                 | 0     |
| 86  | OHX  | 2     | 2082 | 7/7   | 0.91 | 0.17 | 110,110,110,110             | 0     |
| 86  | OHX  | 5     | 4103 | 7/7   | 0.91 | 0.13 | 123,123,123,123             | 0     |
| 86  | OHX  | 1     | 4157 | 7/7   | 0.91 | 0.20 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4107 | 7/7   | 0.91 | 0.19 | 103,103,103,103             | 0     |
| 86  | OHX  | 2     | 2087 | 7/7   | 0.91 | 0.20 | 93,93,93,93                 | 0     |
| 85  | MG   | 2     | 1981 | 1/1   | 0.91 | 0.31 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 4118 | 7/7   | 0.91 | 0.19 | 94,94,94,94                 | 0     |
| 86  | OHX  | 2     | 2100 | 7/7   | 0.91 | 0.17 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3716 | 1/1   | 0.91 | 0.08 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4124 | 7/7   | 0.91 | 0.15 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4126 | 7/7   | 0.91 | 0.18 | 103,103,103,103             | 0     |
| 86  | OHX  | 5     | 4127 | 7/7   | 0.91 | 0.18 | 100,100,100,100             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1982 | 1/1   | 0.91 | 0.24 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4132 | 7/7   | 0.91 | 0.19 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4135 | 7/7   | 0.91 | 0.17 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3579 | 1/1   | 0.91 | 0.27 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3428 | 1/1   | 0.91 | 0.11 | 21,21,21,21                 | 0     |
| 86  | OHX  | 2     | 2122 | 7/7   | 0.91 | 0.16 | 116,116,116,116             | 0     |
| 86  | OHX  | 2     | 2123 | 7/7   | 0.91 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3581 | 1/1   | 0.91 | 0.26 | 36,36,36,36                 | 0     |
| 86  | OHX  | 2     | 2127 | 7/7   | 0.91 | 0.15 | 115,115,115,115             | 0     |
| 86  | OHX  | 5     | 4143 | 7/7   | 0.91 | 0.20 | 106,106,106,106             | 0     |
| 85  | MG   | 5     | 3583 | 1/1   | 0.91 | 0.30 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3585 | 1/1   | 0.91 | 0.21 | 20,20,20,20                 | 0     |
| 85  | MG   | 6     | 1903 | 1/1   | 0.91 | 0.28 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3531 | 1/1   | 0.91 | 0.18 | 19,19,19,19                 | 0     |
| 85  | MG   | 1     | 3536 | 1/1   | 0.91 | 0.35 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1922 | 1/1   | 0.91 | 0.31 | 55,55,55,55                 | 0     |
| 85  | MG   | 1     | 3656 | 1/1   | 0.91 | 0.19 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3802 | 1/1   | 0.91 | 0.16 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3785 | 1/1   | 0.91 | 0.07 | 31,31,31,31                 | 0     |
| 85  | MG   | 3     | 204  | 1/1   | 0.91 | 0.43 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1984 | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 85  | MG   | 5     | 3790 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 86  | OHX  | 2     | 2147 | 7/7   | 0.91 | 0.16 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3603 | 1/1   | 0.91 | 0.07 | 19,19,19,19                 | 0     |
| 86  | OHX  | 5     | 4161 | 7/7   | 0.91 | 0.22 | 94,94,94,94                 | 0     |
| 85  | MG   | 2     | 1908 | 1/1   | 0.91 | 0.26 | 60,60,60,60                 | 0     |
| 85  | MG   | 5     | 3795 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 2004 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 4165 | 7/7   | 0.91 | 0.18 | 102,102,102,102             | 0     |
| 85  | MG   | 5     | 3609 | 1/1   | 0.91 | 0.11 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3610 | 1/1   | 0.91 | 0.20 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4168 | 7/7   | 0.91 | 0.11 | 154,154,154,154             | 0     |
| 85  | MG   | 5     | 3613 | 1/1   | 0.91 | 0.25 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3439 | 1/1   | 0.91 | 0.23 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3454 | 1/1   | 0.91 | 0.16 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3813 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3667 | 1/1   | 0.91 | 0.38 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3619 | 1/1   | 0.91 | 0.26 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3457 | 1/1   | 0.91 | 0.21 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3818 | 1/1   | 0.91 | 0.20 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 2009 | 1/1   | 0.91 | 0.07 | 40,40,40,40                 | 0     |
| 85  | MG   | 6     | 2011 | 1/1   | 0.91 | 0.37 | 54,54,54,54                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3831 | 1/1   | 0.91 | 0.15 | 59,59,59,59                 | 0     |
| 85  | MG   | 6     | 1921 | 1/1   | 0.91 | 0.29 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 1922 | 1/1   | 0.91 | 0.35 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3468 | 1/1   | 0.91 | 0.14 | 29,29,29,29                 | 0     |
| 85  | MG   | 2     | 1918 | 1/1   | 0.91 | 0.33 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4187 | 7/7   | 0.91 | 0.19 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3470 | 1/1   | 0.91 | 0.23 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3501 | 1/1   | 0.91 | 0.26 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3645 | 1/1   | 0.91 | 0.29 | 47,47,47,47                 | 0     |
| 85  | MG   | 2     | 1913 | 1/1   | 0.91 | 0.43 | 64,64,64,64                 | 0     |
| 85  | MG   | 1     | 3505 | 1/1   | 0.91 | 0.19 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4212 | 7/7   | 0.91 | 0.22 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3476 | 1/1   | 0.91 | 0.16 | 19,19,19,19                 | 0     |
| 85  | MG   | 4     | 208  | 1/1   | 0.91 | 0.21 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 1929 | 1/1   | 0.91 | 0.25 | 49,49,49,49                 | 0     |
| 86  | OHX  | 3     | 222  | 7/7   | 0.91 | 0.14 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3673 | 1/1   | 0.91 | 0.41 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3480 | 1/1   | 0.91 | 0.17 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3481 | 1/1   | 0.91 | 0.40 | 57,57,57,57                 | 0     |
| 86  | OHX  | 5     | 4206 | 7/7   | 0.91 | 0.15 | 121,121,121,121             | 0     |
| 85  | MG   | 5     | 3483 | 1/1   | 0.91 | 0.10 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3742 | 1/1   | 0.91 | 0.29 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 4003 | 7/7   | 0.91 | 0.20 | 90,90,90,90                 | 0     |
| 85  | MG   | 1     | 3827 | 1/1   | 0.91 | 0.15 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4022 | 7/7   | 0.91 | 0.16 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3674 | 1/1   | 0.91 | 0.16 | 33,33,33,33                 | 0     |
| 85  | MG   | 2     | 1916 | 1/1   | 0.91 | 0.30 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4039 | 7/7   | 0.91 | 0.18 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3623 | 1/1   | 0.91 | 0.18 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3869 | 1/1   | 0.91 | 0.21 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3490 | 1/1   | 0.91 | 0.33 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3680 | 1/1   | 0.91 | 0.41 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3678 | 1/1   | 0.91 | 0.13 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4074 | 7/7   | 0.91 | 0.15 | 105,105,105,105             | 0     |
| 86  | OHX  | 6     | 2117 | 7/7   | 0.91 | 0.17 | 108,108,108,108             | 0     |
| 86  | OHX  | 6     | 2127 | 7/7   | 0.91 | 0.18 | 98,98,98,98                 | 0     |
| 86  | OHX  | 1     | 4079 | 7/7   | 0.91 | 0.18 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 4081 | 7/7   | 0.91 | 0.21 | 96,96,96,96                 | 0     |
| 86  | OHX  | 6     | 2140 | 7/7   | 0.91 | 0.18 | 111,111,111,111             | 0     |
| 86  | OHX  | 6     | 2143 | 7/7   | 0.91 | 0.15 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3680 | 1/1   | 0.91 | 0.07 | 30,30,30,30                 | 0     |
| 86  | OHX  | 6     | 2145 | 7/7   | 0.91 | 0.17 | 110,110,110,110             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 6     | 2146 | 7/7   | 0.91 | 0.16 | 109,109,109,109             | 0     |
| 86  | OHX  | 6     | 2147 | 7/7   | 0.91 | 0.22 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3688 | 1/1   | 0.91 | 0.12 | 33,33,33,33                 | 0     |
| 86  | OHX  | 6     | 2151 | 7/7   | 0.91 | 0.20 | 92,92,92,92                 | 0     |
| 85  | MG   | 1     | 3681 | 1/1   | 0.91 | 0.15 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 4087 | 7/7   | 0.91 | 0.15 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3883 | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 1944 | 1/1   | 0.91 | 0.41 | 50,50,50,50                 | 0     |
| 86  | OHX  | 6     | 2157 | 7/7   | 0.91 | 0.19 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 1947 | 1/1   | 0.91 | 0.31 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3416 | 1/1   | 0.91 | 0.11 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 4097 | 7/7   | 0.91 | 0.15 | 115,115,115,115             | 0     |
| 86  | OHX  | 6     | 2161 | 7/7   | 0.91 | 0.19 | 101,101,101,101             | 0     |
| 85  | MG   | 2     | 1921 | 1/1   | 0.91 | 0.32 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3700 | 1/1   | 0.91 | 0.17 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 4100 | 7/7   | 0.91 | 0.16 | 116,116,116,116             | 0     |
| 86  | OHX  | 6     | 2166 | 7/7   | 0.91 | 0.15 | 115,115,115,115             | 0     |
| 85  | MG   | L4    | 401  | 1/1   | 0.91 | 0.10 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3890 | 1/1   | 0.91 | 0.07 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3449 | 1/1   | 0.91 | 0.12 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 4105 | 7/7   | 0.91 | 0.18 | 101,101,101,101             | 0     |
| 86  | OHX  | 6     | 2171 | 7/7   | 0.91 | 0.22 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3704 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4107 | 7/7   | 0.91 | 0.20 | 98,98,98,98                 | 0     |
| 86  | OHX  | 8     | 226  | 7/7   | 0.91 | 0.16 | 115,115,115,115             | 0     |
| 86  | OHX  | 1     | 4108 | 7/7   | 0.91 | 0.20 | 97,97,97,97                 | 0     |
| 85  | MG   | 2     | 1937 | 1/1   | 0.91 | 0.29 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3706 | 1/1   | 0.91 | 0.20 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 4114 | 7/7   | 0.91 | 0.25 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3845 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3517 | 1/1   | 0.91 | 0.22 | 22,22,22,22                 | 0     |
| 85  | MG   | 7     | 203  | 1/1   | 0.91 | 0.24 | 43,43,43,43                 | 0     |
| 86  | OHX  | 15    | 305  | 7/7   | 0.91 | 0.17 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3716 | 1/1   | 0.91 | 0.20 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4120 | 7/7   | 0.91 | 0.17 | 105,105,105,105             | 0     |
| 86  | OHX  | 1     | 4121 | 7/7   | 0.91 | 0.18 | 102,102,102,102             | 0     |
| 85  | MG   | 7     | 207  | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 85  | MG   | 7     | 208  | 1/1   | 0.91 | 0.22 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3848 | 1/1   | 0.91 | 0.26 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3532 | 1/1   | 0.91 | 0.17 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3578 | 1/1   | 0.91 | 0.25 | 20,20,20,20                 | 0     |
| 85  | MG   | 1     | 3632 | 1/1   | 0.91 | 0.21 | 50,50,50,50                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3581 | 1/1   | 0.91 | 0.11 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3725 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 86  | OHX  | s4    | 301  | 7/7   | 0.92 | 0.16 | 122,122,122,122             | 0     |
| 86  | OHX  | 2     | 2117 | 7/7   | 0.92 | 0.15 | 110,110,110,110             | 0     |
| 86  | OHX  | 2     | 2119 | 7/7   | 0.92 | 0.15 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3482 | 1/1   | 0.92 | 0.28 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3638 | 1/1   | 0.92 | 0.19 | 29,29,29,29                 | 0     |
| 85  | MG   | 6     | 1949 | 1/1   | 0.92 | 0.28 | 40,40,40,40                 | 0     |
| 86  | OHX  | sR    | 401  | 7/7   | 0.92 | 0.13 | 135,135,135,135             | 0     |
| 85  | MG   | 1     | 3555 | 1/1   | 0.92 | 0.31 | 25,25,25,25                 | 0     |
| 86  | OHX  | 5     | 3999 | 7/7   | 0.92 | 0.15 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 4006 | 7/7   | 0.92 | 0.16 | 87,87,87,87                 | 0     |
| 86  | OHX  | 2     | 2126 | 7/7   | 0.92 | 0.18 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4156 | 7/7   | 0.92 | 0.19 | 105,105,105,105             | 0     |
| 85  | MG   | 1     | 3699 | 1/1   | 0.92 | 0.22 | 31,31,31,31                 | 0     |
| 86  | OHX  | 5     | 4042 | 7/7   | 0.92 | 0.16 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 4043 | 7/7   | 0.92 | 0.18 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3768 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 86  | OHX  | 2     | 2129 | 7/7   | 0.92 | 0.15 | 121,121,121,121             | 0     |
| 86  | OHX  | 5     | 4071 | 7/7   | 0.92 | 0.19 | 106,106,106,106             | 0     |
| 86  | OHX  | 5     | 4075 | 7/7   | 0.92 | 0.20 | 91,91,91,91                 | 0     |
| 86  | OHX  | 2     | 2133 | 7/7   | 0.92 | 0.15 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4092 | 7/7   | 0.92 | 0.19 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 4095 | 7/7   | 0.92 | 0.15 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3804 | 1/1   | 0.92 | 0.09 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3497 | 1/1   | 0.92 | 0.17 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3807 | 1/1   | 0.92 | 0.15 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3850 | 1/1   | 0.92 | 0.26 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4102 | 7/7   | 0.92 | 0.20 | 82,82,82,82                 | 0     |
| 85  | MG   | 5     | 3810 | 1/1   | 0.92 | 0.15 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4104 | 7/7   | 0.92 | 0.17 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3415 | 1/1   | 0.92 | 0.07 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4106 | 7/7   | 0.92 | 0.20 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3652 | 1/1   | 0.92 | 0.26 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3492 | 1/1   | 0.92 | 0.06 | 22,22,22,22                 | 0     |
| 85  | MG   | 2     | 1962 | 1/1   | 0.92 | 0.24 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4115 | 7/7   | 0.92 | 0.14 | 118,118,118,118             | 0     |
| 86  | OHX  | 5     | 4117 | 7/7   | 0.92 | 0.17 | 96,96,96,96                 | 0     |
| 85  | MG   | 6     | 1961 | 1/1   | 0.92 | 0.36 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4119 | 7/7   | 0.92 | 0.18 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4121 | 7/7   | 0.92 | 0.17 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3821 | 1/1   | 0.92 | 0.22 | 32,32,32,32                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3657 | 1/1   | 0.92 | 0.13 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3823 | 1/1   | 0.92 | 0.23 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1935 | 1/1   | 0.92 | 0.31 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3658 | 1/1   | 0.92 | 0.26 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3499 | 1/1   | 0.92 | 0.23 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3855 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4133 | 7/7   | 0.92 | 0.18 | 102,102,102,102             | 0     |
| 85  | MG   | 1     | 3418 | 1/1   | 0.92 | 0.26 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3668 | 1/1   | 0.92 | 0.08 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3670 | 1/1   | 0.92 | 0.30 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3504 | 1/1   | 0.92 | 0.20 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3673 | 1/1   | 0.92 | 0.29 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3507 | 1/1   | 0.92 | 0.24 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4141 | 7/7   | 0.92 | 0.17 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3513 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3850 | 1/1   | 0.92 | 0.09 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3660 | 1/1   | 0.92 | 0.22 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3515 | 1/1   | 0.92 | 0.20 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3714 | 1/1   | 0.92 | 0.08 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3621 | 1/1   | 0.92 | 0.08 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3524 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3685 | 1/1   | 0.92 | 0.16 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3664 | 1/1   | 0.92 | 0.06 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3567 | 1/1   | 0.92 | 0.27 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3577 | 1/1   | 0.92 | 0.12 | 17,17,17,17                 | 0     |
| 86  | OHX  | 2     | 2171 | 7/7   | 0.92 | 0.16 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3692 | 1/1   | 0.92 | 0.11 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3793 | 1/1   | 0.92 | 0.15 | 73,73,73,73                 | 0     |
| 85  | MG   | 5     | 3695 | 1/1   | 0.92 | 0.20 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3867 | 1/1   | 0.92 | 0.31 | 31,31,31,31                 | 0     |
| 86  | OHX  | 5     | 4160 | 7/7   | 0.92 | 0.21 | 93,93,93,93                 | 0     |
| 85  | MG   | N8    | 202  | 1/1   | 0.92 | 0.09 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3794 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3866 | 1/1   | 0.92 | 0.24 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3410 | 1/1   | 0.92 | 0.29 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3867 | 1/1   | 0.92 | 0.08 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3534 | 1/1   | 0.92 | 0.24 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3797 | 1/1   | 0.92 | 0.08 | 16,16,16,16                 | 0     |
| 85  | MG   | 1     | 3535 | 1/1   | 0.92 | 0.24 | 41,41,41,41                 | 0     |
| 86  | OHX  | C5    | 201  | 7/7   | 0.92 | 0.13 | 136,136,136,136             | 0     |
| 86  | OHX  | 1     | 3957 | 7/7   | 0.92 | 0.20 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3967 | 7/7   | 0.92 | 0.18 | 82,82,82,82                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3970 | 7/7   | 0.92 | 0.13 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3981 | 7/7   | 0.92 | 0.23 | 79,79,79,79                 | 0     |
| 86  | OHX  | 3     | 223  | 7/7   | 0.92 | 0.20 | 96,96,96,96                 | 0     |
| 85  | MG   | 2     | 1979 | 1/1   | 0.92 | 0.28 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4007 | 7/7   | 0.92 | 0.20 | 90,90,90,90                 | 0     |
| 86  | OHX  | 1     | 4012 | 7/7   | 0.92 | 0.17 | 101,101,101,101             | 0     |
| 86  | OHX  | 4     | 226  | 7/7   | 0.92 | 0.18 | 91,91,91,91                 | 0     |
| 86  | OHX  | 4     | 229  | 7/7   | 0.92 | 0.13 | 121,121,121,121             | 0     |
| 86  | OHX  | 1     | 4014 | 7/7   | 0.92 | 0.17 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 4015 | 7/7   | 0.92 | 0.15 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3709 | 1/1   | 0.92 | 0.21 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3551 | 1/1   | 0.92 | 0.32 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3713 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3460 | 1/1   | 0.92 | 0.21 | 26,26,26,26                 | 0     |
| 85  | MG   | 2     | 2016 | 1/1   | 0.92 | 0.40 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 4045 | 7/7   | 0.92 | 0.18 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4053 | 7/7   | 0.92 | 0.20 | 87,87,87,87                 | 0     |
| 86  | OHX  | 5     | 4192 | 7/7   | 0.92 | 0.13 | 135,135,135,135             | 0     |
| 85  | MG   | 5     | 3423 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3630 | 1/1   | 0.92 | 0.07 | 21,21,21,21                 | 0     |
| 85  | MG   | 5     | 3425 | 1/1   | 0.92 | 0.15 | 30,30,30,30                 | 0     |
| 86  | OHX  | O3    | 202  | 7/7   | 0.92 | 0.21 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 3676 | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 86  | OHX  | 6     | 2095 | 7/7   | 0.92 | 0.16 | 100,100,100,100             | 0     |
| 85  | MG   | 6     | 1998 | 1/1   | 0.92 | 0.21 | 49,49,49,49                 | 0     |
| 86  | OHX  | 6     | 2107 | 7/7   | 0.92 | 0.18 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3735 | 1/1   | 0.92 | 0.29 | 55,55,55,55                 | 0     |
| 86  | OHX  | 6     | 2125 | 7/7   | 0.92 | 0.17 | 106,106,106,106             | 0     |
| 86  | OHX  | 1     | 4075 | 7/7   | 0.92 | 0.15 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2133 | 7/7   | 0.92 | 0.13 | 126,126,126,126             | 0     |
| 85  | MG   | 1     | 3588 | 1/1   | 0.92 | 0.21 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 4080 | 7/7   | 0.92 | 0.16 | 106,106,106,106             | 0     |
| 86  | OHX  | 6     | 2138 | 7/7   | 0.92 | 0.16 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 4252 | 1/1   | 0.92 | 0.18 | 25,25,25,25                 | 0     |
| 85  | MG   | 7     | 201  | 1/1   | 0.92 | 0.37 | 36,36,36,36                 | 0     |
| 85  | MG   | 2     | 2017 | 1/1   | 0.92 | 0.40 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3679 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3424 | 1/1   | 0.92 | 0.14 | 37,37,37,37                 | 0     |
| 85  | MG   | 7     | 206  | 1/1   | 0.92 | 0.11 | 36,36,36,36                 | 0     |
| 85  | MG   | 2     | 2184 | 1/1   | 0.92 | 0.14 | 78,78,78,78                 | 0     |
| 86  | OHX  | 6     | 2150 | 7/7   | 0.92 | 0.15 | 115,115,115,115             | 0     |
| 85  | MG   | 2     | 1936 | 1/1   | 0.92 | 0.36 | 42,42,42,42                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3736 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 85  | MG   | 7     | 210  | 1/1   | 0.92 | 0.13 | 28,28,28,28                 | 0     |
| 85  | MG   | 4     | 205  | 1/1   | 0.92 | 0.24 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3443 | 1/1   | 0.92 | 0.21 | 20,20,20,20                 | 0     |
| 85  | MG   | 1     | 3749 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 85  | MG   | 6     | 2010 | 1/1   | 0.92 | 0.07 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4102 | 7/7   | 0.92 | 0.21 | 90,90,90,90                 | 0     |
| 85  | MG   | 4     | 209  | 1/1   | 0.92 | 0.11 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3744 | 1/1   | 0.92 | 0.06 | 25,25,25,25                 | 0     |
| 86  | OHX  | 6     | 2162 | 7/7   | 0.92 | 0.20 | 96,96,96,96                 | 0     |
| 85  | MG   | 2     | 1971 | 1/1   | 0.92 | 0.33 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3606 | 1/1   | 0.92 | 0.09 | 42,42,42,42                 | 0     |
| 85  | MG   | 8     | 207  | 1/1   | 0.92 | 0.09 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3458 | 1/1   | 0.92 | 0.20 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3595 | 1/1   | 0.92 | 0.28 | 27,27,27,27                 | 0     |
| 86  | OHX  | 1     | 4112 | 7/7   | 0.92 | 0.17 | 102,102,102,102             | 0     |
| 85  | MG   | 6     | 2016 | 1/1   | 0.92 | 0.12 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3757 | 1/1   | 0.92 | 0.25 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3462 | 1/1   | 0.92 | 0.23 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3549 | 1/1   | 0.92 | 0.22 | 27,27,27,27                 | 0     |
| 85  | MG   | 6     | 1931 | 1/1   | 0.92 | 0.40 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 4118 | 7/7   | 0.92 | 0.20 | 95,95,95,95                 | 0     |
| 85  | MG   | 6     | 2019 | 1/1   | 0.92 | 0.32 | 48,48,48,48                 | 0     |
| 85  | MG   | m4    | 201  | 1/1   | 0.92 | 0.23 | 46,46,46,46                 | 0     |
| 85  | MG   | 4     | 213  | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3608 | 1/1   | 0.92 | 0.17 | 29,29,29,29                 | 0     |
| 85  | MG   | n0    | 202  | 1/1   | 0.92 | 0.11 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3451 | 1/1   | 0.92 | 0.26 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3834 | 1/1   | 0.92 | 0.25 | 16,16,16,16                 | 0     |
| 86  | OHX  | 7     | 226  | 7/7   | 0.92 | 0.21 | 92,92,92,92                 | 0     |
| 85  | MG   | 6     | 2023 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4127 | 7/7   | 0.92 | 0.14 | 120,120,120,120             | 0     |
| 85  | MG   | 1     | 3525 | 1/1   | 0.92 | 0.20 | 20,20,20,20                 | 0     |
| 85  | MG   | 6     | 2026 | 1/1   | 0.92 | 0.11 | 69,69,69,69                 | 0     |
| 85  | MG   | n9    | 3801 | 1/1   | 0.92 | 0.07 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3777 | 1/1   | 0.92 | 0.18 | 45,45,45,45                 | 0     |
| 85  | MG   | o3    | 201  | 1/1   | 0.92 | 0.18 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3648 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3760 | 1/1   | 0.92 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 6     | 1940 | 1/1   | 0.92 | 0.48 | 70,70,70,70                 | 0     |
| 85  | MG   | 5     | 3625 | 1/1   | 0.92 | 0.16 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3691 | 1/1   | 0.92 | 0.12 | 28,28,28,28                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2089 | 7/7   | 0.92 | 0.17 | 100,100,100,100             | 0     |
| 86  | OHX  | 2     | 2093 | 7/7   | 0.92 | 0.23 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3784 | 1/1   | 0.92 | 0.21 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3629 | 1/1   | 0.92 | 0.15 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2103 | 7/7   | 0.92 | 0.16 | 112,112,112,112             | 0     |
| 86  | OHX  | 2     | 2104 | 7/7   | 0.92 | 0.11 | 169,169,169,169             | 0     |
| 86  | OHX  | 2     | 2105 | 7/7   | 0.92 | 0.17 | 97,97,97,97                 | 0     |
| 86  | OHX  | 6     | 2201 | 7/7   | 0.92 | 0.17 | 116,116,116,116             | 0     |
| 85  | MG   | 6     | 1942 | 1/1   | 0.92 | 0.20 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3610 | 1/1   | 0.92 | 0.18 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3697 | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 86  | OHX  | 2     | 2145 | 7/7   | 0.93 | 0.11 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3518 | 1/1   | 0.93 | 0.32 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3701 | 1/1   | 0.93 | 0.07 | 34,34,34,34                 | 0     |
| 85  | MG   | M3    | 202  | 1/1   | 0.93 | 0.10 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3848 | 1/1   | 0.93 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3702 | 1/1   | 0.93 | 0.19 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4079 | 7/7   | 0.93 | 0.17 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4084 | 7/7   | 0.93 | 0.13 | 112,112,112,112             | 0     |
| 86  | OHX  | 5     | 4087 | 7/7   | 0.93 | 0.15 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3530 | 1/1   | 0.93 | 0.30 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3684 | 1/1   | 0.93 | 0.25 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3523 | 1/1   | 0.93 | 0.21 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3687 | 1/1   | 0.93 | 0.18 | 45,45,45,45                 | 0     |
| 86  | OHX  | 5     | 4097 | 7/7   | 0.93 | 0.19 | 93,93,93,93                 | 0     |
| 85  | MG   | 1     | 3494 | 1/1   | 0.93 | 0.18 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3535 | 1/1   | 0.93 | 0.24 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4100 | 7/7   | 0.93 | 0.16 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3776 | 1/1   | 0.93 | 0.26 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3706 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3653 | 1/1   | 0.93 | 0.19 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3556 | 1/1   | 0.93 | 0.26 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3864 | 1/1   | 0.93 | 0.29 | 52,52,52,52                 | 0     |
| 85  | MG   | M7    | 204  | 1/1   | 0.93 | 0.07 | 27,27,27,27                 | 0     |
| 85  | MG   | M7    | 205  | 1/1   | 0.93 | 0.07 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3783 | 1/1   | 0.93 | 0.17 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3414 | 1/1   | 0.93 | 0.20 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4110 | 7/7   | 0.93 | 0.16 | 103,103,103,103             | 0     |
| 86  | OHX  | 5     | 4111 | 7/7   | 0.93 | 0.17 | 104,104,104,104             | 0     |
| 86  | OHX  | 5     | 4113 | 7/7   | 0.93 | 0.19 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 4114 | 7/7   | 0.93 | 0.18 | 95,95,95,95                 | 0     |
| 85  | MG   | 1     | 3859 | 1/1   | 0.93 | 0.18 | 54,54,54,54                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3870 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |
| 85  | MG   | N3    | 202  | 1/1   | 0.93 | 0.21 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 1977 | 1/1   | 0.93 | 0.20 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3558 | 1/1   | 0.93 | 0.23 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3421 | 1/1   | 0.93 | 0.16 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3878 | 1/1   | 0.93 | 0.16 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3612 | 1/1   | 0.93 | 0.11 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3711 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4196 | 7/7   | 0.93 | 0.13 | 149,149,149,149             | 0     |
| 86  | OHX  | 5     | 4128 | 7/7   | 0.93 | 0.15 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3438 | 1/1   | 0.93 | 0.14 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3562 | 1/1   | 0.93 | 0.27 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3715 | 1/1   | 0.93 | 0.13 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4134 | 7/7   | 0.93 | 0.19 | 99,99,99,99                 | 0     |
| 85  | MG   | 6     | 1985 | 1/1   | 0.93 | 0.24 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3423 | 1/1   | 0.93 | 0.13 | 28,28,28,28                 | 0     |
| 85  | MG   | O4    | 201  | 1/1   | 0.93 | 0.21 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3572 | 1/1   | 0.93 | 0.36 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3574 | 1/1   | 0.93 | 0.31 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3792 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 86  | OHX  | D9    | 102  | 7/7   | 0.93 | 0.15 | 109,109,109,109             | 0     |
| 86  | OHX  | 1     | 3915 | 7/7   | 0.93 | 0.19 | 73,73,73,73                 | 0     |
| 86  | OHX  | 1     | 3956 | 7/7   | 0.93 | 0.14 | 86,86,86,86                 | 0     |
| 85  | MG   | 1     | 3463 | 1/1   | 0.93 | 0.29 | 19,19,19,19                 | 0     |
| 85  | MG   | 1     | 3440 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3728 | 1/1   | 0.93 | 0.15 | 20,20,20,20                 | 0     |
| 85  | MG   | 1     | 3620 | 1/1   | 0.93 | 0.19 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 4001 | 7/7   | 0.93 | 0.15 | 133,133,133,133             | 0     |
| 85  | MG   | 6     | 1993 | 1/1   | 0.93 | 0.19 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 4256 | 1/1   | 0.93 | 0.10 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 4257 | 1/1   | 0.93 | 0.30 | 22,22,22,22                 | 0     |
| 85  | MG   | 6     | 1994 | 1/1   | 0.93 | 0.19 | 51,51,51,51                 | 0     |
| 85  | MG   | 6     | 1905 | 1/1   | 0.93 | 0.27 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3438 | 1/1   | 0.93 | 0.34 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 4220 | 1/1   | 0.93 | 0.10 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3482 | 1/1   | 0.93 | 0.27 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3446 | 1/1   | 0.93 | 0.11 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 4032 | 7/7   | 0.93 | 0.15 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3589 | 1/1   | 0.93 | 0.19 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4040 | 7/7   | 0.93 | 0.13 | 114,114,114,114             | 0     |
| 86  | OHX  | 1     | 4042 | 7/7   | 0.93 | 0.17 | 97,97,97,97                 | 0     |
| 85  | MG   | 1     | 3726 | 1/1   | 0.93 | 0.14 | 33,33,33,33                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3592 | 1/1   | 0.93 | 0.25 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4063 | 7/7   | 0.93 | 0.15 | 102,102,102,102             | 0     |
| 86  | OHX  | 1     | 4064 | 7/7   | 0.93 | 0.12 | 123,123,123,123             | 0     |
| 85  | MG   | 1     | 3669 | 1/1   | 0.93 | 0.11 | 37,37,37,37                 | 0     |
| 85  | MG   | 6     | 1913 | 1/1   | 0.93 | 0.28 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3729 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4070 | 7/7   | 0.93 | 0.20 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3533 | 1/1   | 0.93 | 0.09 | 24,24,24,24                 | 0     |
| 85  | MG   | 3     | 206  | 1/1   | 0.93 | 0.32 | 29,29,29,29                 | 0     |
| 86  | OHX  | 6     | 2077 | 7/7   | 0.93 | 0.17 | 92,92,92,92                 | 0     |
| 86  | OHX  | 6     | 2085 | 7/7   | 0.93 | 0.13 | 109,109,109,109             | 0     |
| 86  | OHX  | 5     | 4178 | 7/7   | 0.93 | 0.13 | 126,126,126,126             | 0     |
| 86  | OHX  | 6     | 2091 | 7/7   | 0.93 | 0.18 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3750 | 1/1   | 0.93 | 0.09 | 34,34,34,34                 | 0     |
| 85  | MG   | 8     | 204  | 1/1   | 0.93 | 0.17 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 4076 | 7/7   | 0.93 | 0.34 | 81,81,81,81                 | 0     |
| 85  | MG   | 3     | 207  | 1/1   | 0.93 | 0.34 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3754 | 1/1   | 0.93 | 0.19 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3569 | 1/1   | 0.93 | 0.25 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 4083 | 7/7   | 0.93 | 0.18 | 100,100,100,100             | 0     |
| 86  | OHX  | 6     | 2134 | 7/7   | 0.93 | 0.15 | 101,101,101,101             | 0     |
| 85  | MG   | 6     | 1919 | 1/1   | 0.93 | 0.27 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3807 | 1/1   | 0.93 | 0.12 | 26,26,26,26                 | 0     |
| 85  | MG   | 8     | 210  | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 86  | OHX  | 6     | 2139 | 7/7   | 0.93 | 0.17 | 106,106,106,106             | 0     |
| 85  | MG   | 8     | 211  | 1/1   | 0.93 | 0.11 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 4088 | 7/7   | 0.93 | 0.16 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 4090 | 7/7   | 0.93 | 0.15 | 102,102,102,102             | 0     |
| 85  | MG   | 1     | 3571 | 1/1   | 0.93 | 0.29 | 35,35,35,35                 | 0     |
| 85  | MG   | 13    | 401  | 1/1   | 0.93 | 0.29 | 22,22,22,22                 | 0     |
| 85  | MG   | 15    | 301  | 1/1   | 0.93 | 0.23 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4095 | 7/7   | 0.93 | 0.20 | 95,95,95,95                 | 0     |
| 86  | OHX  | 6     | 2149 | 7/7   | 0.93 | 0.19 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3504 | 1/1   | 0.93 | 0.34 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3612 | 1/1   | 0.93 | 0.10 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3810 | 1/1   | 0.93 | 0.23 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3413 | 1/1   | 0.93 | 0.30 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3467 | 1/1   | 0.93 | 0.14 | 38,38,38,38                 | 0     |
| 86  | OHX  | 6     | 2155 | 7/7   | 0.93 | 0.18 | 93,93,93,93                 | 0     |
| 85  | MG   | 1     | 3485 | 1/1   | 0.93 | 0.23 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1927 | 1/1   | 0.93 | 0.28 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3584 | 1/1   | 0.93 | 0.17 | 31,31,31,31                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3621 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 85  | MG   | n3    | 201  | 1/1   | 0.93 | 0.24 | 21,21,21,21                 | 0     |
| 85  | MG   | 5     | 3623 | 1/1   | 0.93 | 0.21 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3511 | 1/1   | 0.93 | 0.14 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3543 | 1/1   | 0.93 | 0.28 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4109 | 7/7   | 0.93 | 0.11 | 120,120,120,120             | 0     |
| 86  | OHX  | 1     | 4110 | 7/7   | 0.93 | 0.18 | 92,92,92,92                 | 0     |
| 85  | MG   | 6     | 2024 | 1/1   | 0.93 | 0.17 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3745 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3633 | 1/1   | 0.93 | 0.14 | 35,35,35,35                 | 0     |
| 85  | MG   | n9    | 3802 | 1/1   | 0.93 | 0.18 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3632 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3454 | 1/1   | 0.93 | 0.22 | 30,30,30,30                 | 0     |
| 85  | MG   | o3    | 202  | 1/1   | 0.93 | 0.11 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3589 | 1/1   | 0.93 | 0.28 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3832 | 1/1   | 0.93 | 0.17 | 31,31,31,31                 | 0     |
| 85  | MG   | q0    | 202  | 1/1   | 0.93 | 0.08 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3487 | 1/1   | 0.93 | 0.16 | 27,27,27,27                 | 0     |
| 86  | OHX  | 2     | 2041 | 7/7   | 0.93 | 0.17 | 85,85,85,85                 | 0     |
| 86  | OHX  | 2     | 2069 | 7/7   | 0.93 | 0.12 | 125,125,125,125             | 0     |
| 86  | OHX  | 2     | 2076 | 7/7   | 0.93 | 0.14 | 115,115,115,115             | 0     |
| 85  | MG   | 6     | 1938 | 1/1   | 0.93 | 0.24 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3487 | 1/1   | 0.93 | 0.09 | 23,23,23,23                 | 0     |
| 85  | MG   | 2     | 1958 | 1/1   | 0.93 | 0.30 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3644 | 1/1   | 0.93 | 0.26 | 29,29,29,29                 | 0     |
| 85  | MG   | 6     | 2033 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3489 | 1/1   | 0.93 | 0.17 | 22,22,22,22                 | 0     |
| 85  | MG   | 1     | 3836 | 1/1   | 0.93 | 0.18 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3432 | 1/1   | 0.93 | 0.28 | 36,36,36,36                 | 0     |
| 85  | MG   | 2     | 1953 | 1/1   | 0.93 | 0.21 | 76,76,76,76                 | 0     |
| 85  | MG   | 1     | 3645 | 1/1   | 0.93 | 0.08 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3809 | 1/1   | 0.93 | 0.09 | 62,62,62,62                 | 0     |
| 86  | OHX  | 2     | 2114 | 7/7   | 0.93 | 0.15 | 124,124,124,124             | 0     |
| 85  | MG   | 6     | 1948 | 1/1   | 0.93 | 0.25 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3811 | 1/1   | 0.93 | 0.08 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4139 | 7/7   | 0.93 | 0.17 | 87,87,87,87                 | 0     |
| 86  | OHX  | 7     | 223  | 7/7   | 0.93 | 0.14 | 106,106,106,106             | 0     |
| 86  | OHX  | 2     | 2118 | 7/7   | 0.93 | 0.13 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3694 | 1/1   | 0.93 | 0.12 | 27,27,27,27                 | 0     |
| 85  | MG   | 6     | 1950 | 1/1   | 0.93 | 0.21 | 35,35,35,35                 | 0     |
| 86  | OHX  | 8     | 221  | 7/7   | 0.93 | 0.17 | 95,95,95,95                 | 0     |
| 85  | MG   | 5     | 3659 | 1/1   | 0.93 | 0.24 | 22,22,22,22                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3660 | 1/1   | 0.93 | 0.16 | 39,39,39,39                 | 0     |
| 85  | MG   | L4    | 402  | 1/1   | 0.93 | 0.15 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3819 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3662 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 85  | MG   | 6     | 2043 | 1/1   | 0.93 | 0.19 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3604 | 1/1   | 0.93 | 0.21 | 27,27,27,27                 | 0     |
| 86  | OHX  | 2     | 2130 | 7/7   | 0.93 | 0.12 | 150,150,150,150             | 0     |
| 86  | OHX  | 2     | 2132 | 7/7   | 0.93 | 0.17 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3647 | 1/1   | 0.93 | 0.17 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3826 | 1/1   | 0.93 | 0.06 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3827 | 1/1   | 0.93 | 0.17 | 20,20,20,20                 | 0     |
| 85  | MG   | 5     | 3509 | 1/1   | 0.93 | 0.22 | 22,22,22,22                 | 0     |
| 86  | OHX  | d9    | 102  | 7/7   | 0.93 | 0.14 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3669 | 1/1   | 0.93 | 0.09 | 26,26,26,26                 | 0     |
| 85  | MG   | 6     | 1956 | 1/1   | 0.93 | 0.31 | 38,38,38,38                 | 0     |
| 85  | MG   | 6     | 2205 | 1/1   | 0.93 | 0.23 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3605 | 1/1   | 0.93 | 0.12 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3552 | 1/1   | 0.93 | 0.37 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3840 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 4035 | 7/7   | 0.93 | 0.15 | 102,102,102,102             | 0     |
| 87  | ZN   | q2    | 501  | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3437 | 1/1   | 0.93 | 0.19 | 22,22,22,22                 | 0     |
| 88  | 3H3  | 5     | 4251 | 33/33 | 0.93 | 0.10 | 29,29,29,29                 | 0     |
| 86  | OHX  | 5     | 4116 | 7/7   | 0.94 | 0.19 | 82,82,82,82                 | 0     |
| 86  | OHX  | 6     | 2064 | 7/7   | 0.94 | 0.15 | 80,80,80,80                 | 0     |
| 85  | MG   | 1     | 3442 | 1/1   | 0.94 | 0.16 | 19,19,19,19                 | 0     |
| 85  | MG   | 1     | 3503 | 1/1   | 0.94 | 0.16 | 17,17,17,17                 | 0     |
| 86  | OHX  | 5     | 4120 | 7/7   | 0.94 | 0.12 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3599 | 1/1   | 0.94 | 0.10 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3800 | 1/1   | 0.94 | 0.11 | 35,35,35,35                 | 0     |
| 86  | OHX  | 6     | 2100 | 7/7   | 0.94 | 0.14 | 127,127,127,127             | 0     |
| 85  | MG   | 1     | 3614 | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3694 | 1/1   | 0.94 | 0.06 | 35,35,35,35                 | 0     |
| 86  | OHX  | 6     | 2112 | 7/7   | 0.94 | 0.14 | 99,99,99,99                 | 0     |
| 86  | OHX  | 6     | 2114 | 7/7   | 0.94 | 0.16 | 102,102,102,102             | 0     |
| 86  | OHX  | 5     | 4130 | 7/7   | 0.94 | 0.16 | 95,95,95,95                 | 0     |
| 86  | OHX  | 6     | 2116 | 7/7   | 0.94 | 0.13 | 100,100,100,100             | 0     |
| 85  | MG   | 6     | 1976 | 1/1   | 0.94 | 0.14 | 33,33,33,33                 | 0     |
| 86  | OHX  | 6     | 2122 | 7/7   | 0.94 | 0.13 | 115,115,115,115             | 0     |
| 86  | OHX  | 6     | 2123 | 7/7   | 0.94 | 0.14 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3551 | 1/1   | 0.94 | 0.26 | 25,25,25,25                 | 0     |
| 86  | OHX  | 6     | 2126 | 7/7   | 0.94 | 0.34 | 81,81,81,81                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3430 | 1/1   | 0.94 | 0.27 | 41,41,41,41                 | 0     |
| 86  | OHX  | 6     | 2131 | 7/7   | 0.94 | 0.13 | 119,119,119,119             | 0     |
| 86  | OHX  | 6     | 2132 | 7/7   | 0.94 | 0.15 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3699 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 8     | 201  | 1/1   | 0.94 | 0.28 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3431 | 1/1   | 0.94 | 0.26 | 41,41,41,41                 | 0     |
| 85  | MG   | 6     | 1980 | 1/1   | 0.94 | 0.32 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4144 | 7/7   | 0.94 | 0.19 | 97,97,97,97                 | 0     |
| 86  | OHX  | 6     | 2137 | 7/7   | 0.94 | 0.17 | 101,101,101,101             | 0     |
| 85  | MG   | 1     | 3618 | 1/1   | 0.94 | 0.27 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 1932 | 1/1   | 0.94 | 0.20 | 37,37,37,37                 | 0     |
| 85  | MG   | 2     | 2013 | 1/1   | 0.94 | 0.23 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3520 | 1/1   | 0.94 | 0.18 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3614 | 1/1   | 0.94 | 0.08 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3708 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3523 | 1/1   | 0.94 | 0.26 | 23,23,23,23                 | 0     |
| 85  | MG   | 8     | 212  | 1/1   | 0.94 | 0.22 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3458 | 1/1   | 0.94 | 0.16 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2169 | 7/7   | 0.94 | 0.19 | 96,96,96,96                 | 0     |
| 85  | MG   | 5     | 3445 | 1/1   | 0.94 | 0.24 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3510 | 1/1   | 0.94 | 0.26 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 3528 | 1/1   | 0.94 | 0.25 | 22,22,22,22                 | 0     |
| 85  | MG   | 5     | 3529 | 1/1   | 0.94 | 0.26 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3472 | 1/1   | 0.94 | 0.06 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3474 | 1/1   | 0.94 | 0.20 | 20,20,20,20                 | 0     |
| 85  | MG   | 5     | 3719 | 1/1   | 0.94 | 0.12 | 31,31,31,31                 | 0     |
| 85  | MG   | 4     | 206  | 1/1   | 0.94 | 0.26 | 28,28,28,28                 | 0     |
| 85  | MG   | m7    | 202  | 1/1   | 0.94 | 0.20 | 25,25,25,25                 | 0     |
| 85  | MG   | 4     | 207  | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3435 | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3765 | 1/1   | 0.94 | 0.19 | 40,40,40,40                 | 0     |
| 85  | MG   | 2     | 2004 | 1/1   | 0.94 | 0.12 | 67,67,67,67                 | 0     |
| 85  | MG   | n3    | 202  | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3634 | 1/1   | 0.94 | 0.26 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3841 | 1/1   | 0.94 | 0.27 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3843 | 1/1   | 0.94 | 0.09 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 3924 | 7/7   | 0.94 | 0.16 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3932 | 7/7   | 0.94 | 0.17 | 82,82,82,82                 | 0     |
| 85  | MG   | 5     | 3543 | 1/1   | 0.94 | 0.13 | 23,23,23,23                 | 0     |
| 85  | MG   | O7    | 102  | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3463 | 1/1   | 0.94 | 0.26 | 44,44,44,44                 | 0     |
| 85  | MG   | 6     | 1946 | 1/1   | 0.94 | 0.30 | 52,52,52,52                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3595 | 1/1   | 0.94 | 0.24 | 22,22,22,22                 | 0     |
| 86  | OHX  | 1     | 3984 | 7/7   | 0.94 | 0.16 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4000 | 7/7   | 0.94 | 0.19 | 82,82,82,82                 | 0     |
| 85  | MG   | 1     | 3815 | 1/1   | 0.94 | 0.07 | 26,26,26,26                 | 0     |
| 85  | MG   | 6     | 2002 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 85  | MG   | s8    | 302  | 1/1   | 0.94 | 0.11 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 4008 | 7/7   | 0.94 | 0.15 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 4010 | 7/7   | 0.94 | 0.20 | 82,82,82,82                 | 0     |
| 85  | MG   | 5     | 3853 | 1/1   | 0.94 | 0.11 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3817 | 1/1   | 0.94 | 0.26 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3647 | 1/1   | 0.94 | 0.16 | 41,41,41,41                 | 0     |
| 85  | MG   | q3    | 502  | 1/1   | 0.94 | 0.25 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4021 | 7/7   | 0.94 | 0.14 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3553 | 1/1   | 0.94 | 0.28 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3741 | 1/1   | 0.94 | 0.08 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3541 | 1/1   | 0.94 | 0.19 | 19,19,19,19                 | 0     |
| 86  | OHX  | 2     | 2080 | 7/7   | 0.94 | 0.19 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3859 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3555 | 1/1   | 0.94 | 0.23 | 20,20,20,20                 | 0     |
| 85  | MG   | 1     | 3601 | 1/1   | 0.94 | 0.15 | 18,18,18,18                 | 0     |
| 86  | OHX  | 2     | 2090 | 7/7   | 0.94 | 0.17 | 89,89,89,89                 | 0     |
| 86  | OHX  | 2     | 2092 | 7/7   | 0.94 | 0.15 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4054 | 7/7   | 0.94 | 0.17 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 4057 | 7/7   | 0.94 | 0.14 | 114,114,114,114             | 0     |
| 86  | OHX  | 1     | 4058 | 7/7   | 0.94 | 0.22 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 4061 | 7/7   | 0.94 | 0.17 | 97,97,97,97                 | 0     |
| 85  | MG   | 1     | 3693 | 1/1   | 0.94 | 0.27 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3747 | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3655 | 1/1   | 0.94 | 0.29 | 45,45,45,45                 | 0     |
| 86  | OHX  | 2     | 2101 | 7/7   | 0.94 | 0.14 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3565 | 1/1   | 0.94 | 0.26 | 22,22,22,22                 | 0     |
| 85  | MG   | d3    | 201  | 1/1   | 0.94 | 0.16 | 39,39,39,39                 | 0     |
| 85  | MG   | 6     | 1908 | 1/1   | 0.94 | 0.23 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4072 | 7/7   | 0.94 | 0.18 | 103,103,103,103             | 0     |
| 86  | OHX  | 2     | 2106 | 7/7   | 0.94 | 0.15 | 111,111,111,111             | 0     |
| 86  | OHX  | 2     | 2107 | 7/7   | 0.94 | 0.15 | 96,96,96,96                 | 0     |
| 85  | MG   | sM    | 301  | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 86  | OHX  | 2     | 2109 | 7/7   | 0.94 | 0.12 | 123,123,123,123             | 0     |
| 86  | OHX  | 1     | 4077 | 7/7   | 0.94 | 0.14 | 97,97,97,97                 | 0     |
| 86  | OHX  | 1     | 4078 | 7/7   | 0.94 | 0.16 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 3955 | 7/7   | 0.94 | 0.12 | 79,79,79,79                 | 0     |
| 86  | OHX  | 2     | 2110 | 7/7   | 0.94 | 0.14 | 113,113,113,113             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3461 | 1/1   | 0.94 | 0.20 | 20,20,20,20                 | 0     |
| 85  | MG   | 5     | 3758 | 1/1   | 0.94 | 0.24 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4082 | 7/7   | 0.94 | 0.16 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 4026 | 7/7   | 0.94 | 0.17 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3760 | 1/1   | 0.94 | 0.06 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4030 | 7/7   | 0.94 | 0.16 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 4032 | 7/7   | 0.94 | 0.18 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3822 | 1/1   | 0.94 | 0.18 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3695 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4041 | 7/7   | 0.94 | 0.13 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3573 | 1/1   | 0.94 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | 6     | 2012 | 1/1   | 0.94 | 0.21 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4051 | 7/7   | 0.94 | 0.16 | 88,88,88,88                 | 0     |
| 86  | OHX  | 2     | 2121 | 7/7   | 0.94 | 0.14 | 116,116,116,116             | 0     |
| 85  | MG   | 2     | 1957 | 1/1   | 0.94 | 0.30 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 4069 | 7/7   | 0.94 | 0.13 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3766 | 1/1   | 0.94 | 0.12 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4072 | 7/7   | 0.94 | 0.17 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4073 | 7/7   | 0.94 | 0.16 | 93,93,93,93                 | 0     |
| 86  | OHX  | 2     | 2124 | 7/7   | 0.94 | 0.14 | 116,116,116,116             | 0     |
| 86  | OHX  | 5     | 4076 | 7/7   | 0.94 | 0.16 | 99,99,99,99                 | 0     |
| 86  | OHX  | 3     | 221  | 7/7   | 0.94 | 0.14 | 102,102,102,102             | 0     |
| 86  | OHX  | 7     | 224  | 7/7   | 0.94 | 0.18 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 4083 | 7/7   | 0.94 | 0.16 | 94,94,94,94                 | 0     |
| 85  | MG   | 6     | 2014 | 1/1   | 0.94 | 0.12 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 4094 | 7/7   | 0.94 | 0.11 | 129,129,129,129             | 0     |
| 86  | OHX  | 8     | 219  | 7/7   | 0.94 | 0.19 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 4088 | 7/7   | 0.94 | 0.18 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 3778 | 1/1   | 0.94 | 0.09 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4091 | 7/7   | 0.94 | 0.19 | 92,92,92,92                 | 0     |
| 85  | MG   | 1     | 3779 | 1/1   | 0.94 | 0.14 | 24,24,24,24                 | 0     |
| 86  | OHX  | 5     | 4094 | 7/7   | 0.94 | 0.15 | 101,101,101,101             | 0     |
| 85  | MG   | 2     | 2007 | 1/1   | 0.94 | 0.42 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3772 | 1/1   | 0.94 | 0.12 | 23,23,23,23                 | 0     |
| 86  | OHX  | 4     | 227  | 7/7   | 0.94 | 0.18 | 86,86,86,86                 | 0     |
| 85  | MG   | 1     | 3568 | 1/1   | 0.94 | 0.20 | 19,19,19,19                 | 0     |
| 85  | MG   | 5     | 3582 | 1/1   | 0.94 | 0.31 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3409 | 1/1   | 0.94 | 0.27 | 30,30,30,30                 | 0     |
| 85  | MG   | 2     | 1906 | 1/1   | 0.94 | 0.23 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3420 | 1/1   | 0.94 | 0.24 | 29,29,29,29                 | 0     |
| 85  | MG   | M0    | 302  | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 86  | OHX  | m0    | 301  | 7/7   | 0.94 | 0.14 | 105,105,105,105             | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3574 | 1/1   | 0.94 | 0.29 | 30,30,30,30                 | 0     |
| 86  | OHX  | L3    | 403  | 7/7   | 0.94 | 0.17 | 90,90,90,90                 | 0     |
| 85  | MG   | 1     | 3741 | 1/1   | 0.94 | 0.17 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 4253 | 1/1   | 0.94 | 0.19 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3524 | 1/1   | 0.94 | 0.06 | 20,20,20,20                 | 0     |
| 86  | OHX  | M0    | 303  | 7/7   | 0.94 | 0.15 | 86,86,86,86                 | 0     |
| 85  | MG   | 3     | 205  | 1/1   | 0.94 | 0.23 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3686 | 1/1   | 0.94 | 0.15 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3787 | 1/1   | 0.94 | 0.14 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3427 | 1/1   | 0.94 | 0.17 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3594 | 1/1   | 0.94 | 0.36 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3771 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3575 | 1/1   | 0.95 | 0.23 | 22,22,22,22                 | 0     |
| 85  | MG   | 1     | 3491 | 1/1   | 0.95 | 0.16 | 23,23,23,23                 | 0     |
| 86  | OHX  | 6     | 2098 | 7/7   | 0.95 | 0.12 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3520 | 1/1   | 0.95 | 0.14 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3703 | 1/1   | 0.95 | 0.06 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3777 | 1/1   | 0.95 | 0.16 | 55,55,55,55                 | 0     |
| 86  | OHX  | 6     | 2111 | 7/7   | 0.95 | 0.13 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3806 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3665 | 1/1   | 0.95 | 0.17 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3444 | 1/1   | 0.95 | 0.10 | 21,21,21,21                 | 0     |
| 85  | MG   | 8     | 203  | 1/1   | 0.95 | 0.26 | 37,37,37,37                 | 0     |
| 85  | MG   | 2     | 1903 | 1/1   | 0.95 | 0.30 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3557 | 1/1   | 0.95 | 0.17 | 38,38,38,38                 | 0     |
| 86  | OHX  | 6     | 2124 | 7/7   | 0.95 | 0.15 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3736 | 1/1   | 0.95 | 0.20 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3710 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3449 | 1/1   | 0.95 | 0.37 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 4125 | 7/7   | 0.95 | 0.12 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2128 | 7/7   | 0.95 | 0.12 | 109,109,109,109             | 0     |
| 86  | OHX  | 6     | 2129 | 7/7   | 0.95 | 0.13 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3450 | 1/1   | 0.95 | 0.11 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 4129 | 7/7   | 0.95 | 0.12 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3622 | 1/1   | 0.95 | 0.26 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3817 | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3714 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 1989 | 1/1   | 0.95 | 0.12 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3506 | 1/1   | 0.95 | 0.29 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3533 | 1/1   | 0.95 | 0.22 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3559 | 1/1   | 0.95 | 0.20 | 18,18,18,18                 | 0     |
| 85  | MG   | 5     | 3456 | 1/1   | 0.95 | 0.18 | 21,21,21,21                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3637 | 1/1   | 0.95 | 0.25 | 41,41,41,41                 | 0     |
| 86  | OHX  | 6     | 2141 | 7/7   | 0.95 | 0.11 | 127,127,127,127             | 0     |
| 85  | MG   | 2     | 2001 | 1/1   | 0.95 | 0.18 | 63,63,63,63                 | 0     |
| 85  | MG   | 5     | 3633 | 1/1   | 0.95 | 0.46 | 71,71,71,71                 | 0     |
| 85  | MG   | 5     | 3723 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 85  | MG   | m7    | 201  | 1/1   | 0.95 | 0.16 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3724 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3833 | 1/1   | 0.95 | 0.12 | 26,26,26,26                 | 0     |
| 85  | MG   | m7    | 204  | 1/1   | 0.95 | 0.05 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3459 | 1/1   | 0.95 | 0.11 | 23,23,23,23                 | 0     |
| 85  | MG   | n0    | 201  | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 85  | MG   | 2     | 2006 | 1/1   | 0.95 | 0.19 | 45,45,45,45                 | 0     |
| 85  | MG   | N3    | 201  | 1/1   | 0.95 | 0.25 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3509 | 1/1   | 0.95 | 0.20 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3730 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 85  | MG   | C3    | 201  | 1/1   | 0.95 | 0.39 | 56,56,56,56                 | 0     |
| 85  | MG   | 4     | 203  | 1/1   | 0.95 | 0.32 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3549 | 1/1   | 0.95 | 0.23 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3791 | 1/1   | 0.95 | 0.15 | 19,19,19,19                 | 0     |
| 85  | MG   | 6     | 1945 | 1/1   | 0.95 | 0.33 | 43,43,43,43                 | 0     |
| 85  | MG   | c8    | 201  | 1/1   | 0.95 | 0.31 | 57,57,57,57                 | 0     |
| 86  | OHX  | 1     | 3939 | 7/7   | 0.95 | 0.14 | 84,84,84,84                 | 0     |
| 86  | OHX  | 1     | 3951 | 7/7   | 0.95 | 0.14 | 72,72,72,72                 | 0     |
| 85  | MG   | 5     | 3849 | 1/1   | 0.95 | 0.16 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3477 | 1/1   | 0.95 | 0.10 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3513 | 1/1   | 0.95 | 0.23 | 18,18,18,18                 | 0     |
| 85  | MG   | 1     | 3401 | 1/1   | 0.95 | 0.29 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 3972 | 7/7   | 0.95 | 0.12 | 107,107,107,107             | 0     |
| 85  | MG   | 5     | 3472 | 1/1   | 0.95 | 0.10 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3563 | 1/1   | 0.95 | 0.19 | 17,17,17,17                 | 0     |
| 86  | OHX  | 1     | 4159 | 7/7   | 0.95 | 0.13 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 4170 | 7/7   | 0.95 | 0.31 | 81,81,81,81                 | 0     |
| 86  | OHX  | 1     | 3992 | 7/7   | 0.95 | 0.15 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3995 | 7/7   | 0.95 | 0.14 | 81,81,81,81                 | 0     |
| 85  | MG   | 6     | 2006 | 1/1   | 0.95 | 0.16 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3709 | 1/1   | 0.95 | 0.14 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3475 | 1/1   | 0.95 | 0.27 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4005 | 7/7   | 0.95 | 0.23 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 4006 | 7/7   | 0.95 | 0.13 | 102,102,102,102             | 0     |
| 86  | OHX  | 2     | 2044 | 7/7   | 0.95 | 0.14 | 96,96,96,96                 | 0     |
| 86  | OHX  | 2     | 2068 | 7/7   | 0.95 | 0.11 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 4009 | 7/7   | 0.95 | 0.14 | 93,93,93,93                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | sM    | 302  | 1/1   | 0.95 | 0.13 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3594 | 1/1   | 0.95 | 0.23 | 22,22,22,22                 | 0     |
| 86  | OHX  | 1     | 4013 | 7/7   | 0.95 | 0.14 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2078 | 7/7   | 0.95 | 0.13 | 100,100,100,100             | 0     |
| 86  | OHX  | 2     | 2079 | 7/7   | 0.95 | 0.12 | 107,107,107,107             | 0     |
| 86  | OHX  | 1     | 4016 | 7/7   | 0.95 | 0.12 | 105,105,105,105             | 0     |
| 86  | OHX  | 1     | 4017 | 7/7   | 0.95 | 0.16 | 97,97,97,97                 | 0     |
| 86  | OHX  | 1     | 4019 | 7/7   | 0.95 | 0.14 | 89,89,89,89                 | 0     |
| 85  | MG   | 1     | 3798 | 1/1   | 0.95 | 0.17 | 39,39,39,39                 | 0     |
| 86  | OHX  | 2     | 2081 | 7/7   | 0.95 | 0.10 | 127,127,127,127             | 0     |
| 85  | MG   | 5     | 3404 | 1/1   | 0.95 | 0.11 | 32,32,32,32                 | 0     |
| 86  | OHX  | 2     | 2086 | 7/7   | 0.95 | 0.12 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 4025 | 7/7   | 0.95 | 0.15 | 91,91,91,91                 | 0     |
| 86  | OHX  | 1     | 4026 | 7/7   | 0.95 | 0.12 | 116,116,116,116             | 0     |
| 86  | OHX  | 5     | 4197 | 7/7   | 0.95 | 0.15 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 4198 | 7/7   | 0.95 | 0.14 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4199 | 7/7   | 0.95 | 0.16 | 98,98,98,98                 | 0     |
| 86  | OHX  | 1     | 4027 | 7/7   | 0.95 | 0.12 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 4029 | 7/7   | 0.95 | 0.13 | 102,102,102,102             | 0     |
| 85  | MG   | 5     | 3751 | 1/1   | 0.95 | 0.25 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3752 | 1/1   | 0.95 | 0.20 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4033 | 7/7   | 0.95 | 0.11 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4035 | 7/7   | 0.95 | 0.15 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 4037 | 7/7   | 0.95 | 0.16 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3571 | 1/1   | 0.95 | 0.26 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3406 | 1/1   | 0.95 | 0.12 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3755 | 1/1   | 0.95 | 0.27 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3754 | 1/1   | 0.95 | 0.06 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4049 | 7/7   | 0.95 | 0.17 | 87,87,87,87                 | 0     |
| 86  | OHX  | c1    | 202  | 7/7   | 0.95 | 0.14 | 108,108,108,108             | 0     |
| 86  | OHX  | 1     | 4050 | 7/7   | 0.95 | 0.17 | 92,92,92,92                 | 0     |
| 86  | OHX  | 2     | 2097 | 7/7   | 0.95 | 0.10 | 131,131,131,131             | 0     |
| 86  | OHX  | 5     | 4215 | 7/7   | 0.95 | 0.16 | 85,85,85,85                 | 0     |
| 86  | OHX  | 2     | 2098 | 7/7   | 0.95 | 0.11 | 126,126,126,126             | 0     |
| 86  | OHX  | 2     | 2099 | 7/7   | 0.95 | 0.17 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3664 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 85  | MG   | 6     | 1953 | 1/1   | 0.95 | 0.33 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 3974 | 7/7   | 0.95 | 0.12 | 89,89,89,89                 | 0     |
| 86  | OHX  | 5     | 3977 | 7/7   | 0.95 | 0.13 | 81,81,81,81                 | 0     |
| 85  | MG   | 1     | 3800 | 1/1   | 0.95 | 0.18 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1973 | 1/1   | 0.95 | 0.19 | 57,57,57,57                 | 0     |
| 85  | MG   | 6     | 1906 | 1/1   | 0.95 | 0.28 | 43,43,43,43                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3874 | 1/1   | 0.95 | 0.40 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4020 | 7/7   | 0.95 | 0.17 | 85,85,85,85                 | 0     |
| 86  | OHX  | 5     | 4023 | 7/7   | 0.95 | 0.16 | 89,89,89,89                 | 0     |
| 85  | MG   | 5     | 3486 | 1/1   | 0.95 | 0.22 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4069 | 7/7   | 0.95 | 0.10 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4029 | 7/7   | 0.95 | 0.22 | 76,76,76,76                 | 0     |
| 85  | MG   | 1     | 3596 | 1/1   | 0.95 | 0.27 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 4232 | 7/7   | 0.95 | 0.24 | 82,82,82,82                 | 0     |
| 85  | MG   | 5     | 3879 | 1/1   | 0.95 | 0.13 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4033 | 7/7   | 0.95 | 0.18 | 85,85,85,85                 | 0     |
| 85  | MG   | 1     | 3715 | 1/1   | 0.95 | 0.05 | 31,31,31,31                 | 0     |
| 86  | OHX  | 5     | 4036 | 7/7   | 0.95 | 0.12 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2111 | 7/7   | 0.95 | 0.15 | 93,93,93,93                 | 0     |
| 85  | MG   | 1     | 3759 | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3675 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 85  | MG   | 4     | 217  | 1/1   | 0.95 | 0.24 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 4048 | 7/7   | 0.95 | 0.14 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 4050 | 7/7   | 0.95 | 0.11 | 111,111,111,111             | 0     |
| 86  | OHX  | 3     | 216  | 7/7   | 0.95 | 0.16 | 87,87,87,87                 | 0     |
| 86  | OHX  | 5     | 4052 | 7/7   | 0.95 | 0.17 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 4053 | 7/7   | 0.95 | 0.25 | 80,80,80,80                 | 0     |
| 86  | OHX  | 5     | 4056 | 7/7   | 0.95 | 0.16 | 87,87,87,87                 | 0     |
| 86  | OHX  | 5     | 4057 | 7/7   | 0.95 | 0.13 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4058 | 7/7   | 0.95 | 0.12 | 109,109,109,109             | 0     |
| 86  | OHX  | 5     | 4061 | 7/7   | 0.95 | 0.23 | 80,80,80,80                 | 0     |
| 85  | MG   | 6     | 1911 | 1/1   | 0.95 | 0.21 | 38,38,38,38                 | 0     |
| 85  | MG   | 4     | 218  | 1/1   | 0.95 | 0.07 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4064 | 7/7   | 0.95 | 0.10 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4067 | 7/7   | 0.95 | 0.12 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3493 | 1/1   | 0.95 | 0.17 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3597 | 1/1   | 0.95 | 0.23 | 22,22,22,22                 | 0     |
| 86  | OHX  | 8     | 218  | 7/7   | 0.95 | 0.12 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3775 | 1/1   | 0.95 | 0.11 | 21,21,21,21                 | 0     |
| 85  | MG   | 1     | 3717 | 1/1   | 0.95 | 0.18 | 56,56,56,56                 | 0     |
| 86  | OHX  | 8     | 223  | 7/7   | 0.95 | 0.14 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3892 | 1/1   | 0.95 | 0.24 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3684 | 1/1   | 0.95 | 0.25 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3591 | 1/1   | 0.95 | 0.20 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4082 | 7/7   | 0.95 | 0.18 | 85,85,85,85                 | 0     |
| 86  | OHX  | 4     | 230  | 7/7   | 0.95 | 0.12 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3779 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4085 | 7/7   | 0.95 | 0.15 | 95,95,95,95                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4086 | 7/7   | 0.95 | 0.16 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3532 | 1/1   | 0.95 | 0.25 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3764 | 1/1   | 0.95 | 0.15 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3452 | 1/1   | 0.95 | 0.13 | 23,23,23,23                 | 0     |
| 85  | MG   | L4    | 403  | 1/1   | 0.95 | 0.07 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 4255 | 1/1   | 0.95 | 0.23 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3690 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3603 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 4258 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3505 | 1/1   | 0.95 | 0.32 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3723 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3572 | 1/1   | 0.95 | 0.22 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3512 | 1/1   | 0.95 | 0.24 | 20,20,20,20                 | 0     |
| 85  | MG   | 7     | 205  | 1/1   | 0.95 | 0.30 | 23,23,23,23                 | 0     |
| 87  | ZN   | Q2    | 501  | 1/1   | 0.95 | 0.14 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3628 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 86  | OHX  | 2     | 2142 | 7/7   | 0.95 | 0.12 | 127,127,127,127             | 0     |
| 85  | MG   | 5     | 3697 | 1/1   | 0.95 | 0.13 | 26,26,26,26                 | 0     |
| 85  | MG   | 2     | 1925 | 1/1   | 0.95 | 0.34 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 3987 | 7/7   | 0.96 | 0.13 | 80,80,80,80                 | 0     |
| 86  | OHX  | 5     | 4112 | 7/7   | 0.96 | 0.29 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 3990 | 7/7   | 0.96 | 0.11 | 97,97,97,97                 | 0     |
| 86  | OHX  | 1     | 3991 | 7/7   | 0.96 | 0.13 | 92,92,92,92                 | 0     |
| 85  | MG   | 5     | 3559 | 1/1   | 0.96 | 0.22 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 3993 | 7/7   | 0.96 | 0.15 | 84,84,84,84                 | 0     |
| 86  | OHX  | 1     | 3994 | 7/7   | 0.96 | 0.14 | 92,92,92,92                 | 0     |
| 85  | MG   | 5     | 3796 | 1/1   | 0.96 | 0.19 | 27,27,27,27                 | 0     |
| 86  | OHX  | 6     | 2142 | 7/7   | 0.96 | 0.13 | 108,108,108,108             | 0     |
| 86  | OHX  | 1     | 3996 | 7/7   | 0.96 | 0.14 | 93,93,93,93                 | 0     |
| 86  | OHX  | 1     | 3997 | 7/7   | 0.96 | 0.11 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3891 | 1/1   | 0.96 | 0.07 | 64,64,64,64                 | 0     |
| 85  | MG   | 5     | 3798 | 1/1   | 0.96 | 0.26 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3799 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 86  | OHX  | 2     | 2096 | 7/7   | 0.96 | 0.11 | 121,121,121,121             | 0     |
| 85  | MG   | 1     | 3775 | 1/1   | 0.96 | 0.08 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3657 | 1/1   | 0.96 | 0.11 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3710 | 1/1   | 0.96 | 0.06 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3403 | 1/1   | 0.96 | 0.19 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3439 | 1/1   | 0.96 | 0.14 | 24,24,24,24                 | 0     |
| 86  | OHX  | 1     | 4011 | 7/7   | 0.96 | 0.14 | 89,89,89,89                 | 0     |
| 85  | MG   | 5     | 3440 | 1/1   | 0.96 | 0.16 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 4254 | 1/1   | 0.96 | 0.25 | 19,19,19,19                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3743 | 1/1   | 0.96 | 0.20 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3823 | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 4158 | 7/7   | 0.96 | 0.16 | 84,84,84,84                 | 0     |
| 85  | MG   | L2    | 301  | 1/1   | 0.96 | 0.05 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3651 | 1/1   | 0.96 | 0.06 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3726 | 1/1   | 0.96 | 0.12 | 31,31,31,31                 | 0     |
| 85  | MG   | L3    | 401  | 1/1   | 0.96 | 0.16 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3501 | 1/1   | 0.96 | 0.19 | 30,30,30,30                 | 0     |
| 85  | MG   | 6     | 1954 | 1/1   | 0.96 | 0.29 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4023 | 7/7   | 0.96 | 0.14 | 93,93,93,93                 | 0     |
| 86  | OHX  | 2     | 2113 | 7/7   | 0.96 | 0.12 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3600 | 1/1   | 0.96 | 0.21 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 3815 | 1/1   | 0.96 | 0.18 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3539 | 1/1   | 0.96 | 0.21 | 17,17,17,17                 | 0     |
| 85  | MG   | 1     | 3747 | 1/1   | 0.96 | 0.13 | 22,22,22,22                 | 0     |
| 86  | OHX  | 1     | 4030 | 7/7   | 0.96 | 0.11 | 103,103,103,103             | 0     |
| 85  | MG   | 5     | 3508 | 1/1   | 0.96 | 0.28 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3748 | 1/1   | 0.96 | 0.16 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3510 | 1/1   | 0.96 | 0.06 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 4153 | 7/7   | 0.96 | 0.15 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 4034 | 7/7   | 0.96 | 0.14 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3511 | 1/1   | 0.96 | 0.30 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3602 | 1/1   | 0.96 | 0.14 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 4038 | 7/7   | 0.96 | 0.10 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 4222 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3830 | 1/1   | 0.96 | 0.07 | 16,16,16,16                 | 0     |
| 86  | OHX  | 1     | 4041 | 7/7   | 0.96 | 0.15 | 85,85,85,85                 | 0     |
| 85  | MG   | 6     | 1962 | 1/1   | 0.96 | 0.16 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3540 | 1/1   | 0.96 | 0.35 | 48,48,48,48                 | 0     |
| 86  | OHX  | 1     | 4047 | 7/7   | 0.96 | 0.14 | 85,85,85,85                 | 0     |
| 85  | MG   | 5     | 3830 | 1/1   | 0.96 | 0.13 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3640 | 1/1   | 0.96 | 0.06 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4051 | 7/7   | 0.96 | 0.13 | 99,99,99,99                 | 0     |
| 85  | MG   | 6     | 1965 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 86  | OHX  | 2     | 2131 | 7/7   | 0.96 | 0.15 | 93,93,93,93                 | 0     |
| 86  | OHX  | 1     | 4055 | 7/7   | 0.96 | 0.13 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 4056 | 7/7   | 0.96 | 0.11 | 112,112,112,112             | 0     |
| 86  | OHX  | 5     | 4171 | 7/7   | 0.96 | 0.33 | 73,73,73,73                 | 0     |
| 85  | MG   | 5     | 3461 | 1/1   | 0.96 | 0.05 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3522 | 1/1   | 0.96 | 0.25 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4059 | 7/7   | 0.96 | 0.12 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3466 | 1/1   | 0.96 | 0.28 | 49,49,49,49                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4062 | 7/7   | 0.96 | 0.09 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3838 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3642 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3525 | 1/1   | 0.96 | 0.21 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3755 | 1/1   | 0.96 | 0.14 | 18,18,18,18                 | 0     |
| 86  | OHX  | 6     | 2202 | 7/7   | 0.96 | 0.08 | 159,159,159,159             | 0     |
| 85  | MG   | 8     | 213  | 1/1   | 0.96 | 0.31 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3842 | 1/1   | 0.96 | 0.20 | 42,42,42,42                 | 0     |
| 85  | MG   | 12    | 302  | 1/1   | 0.96 | 0.10 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3677 | 1/1   | 0.96 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3586 | 1/1   | 0.96 | 0.32 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3441 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3601 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3839 | 1/1   | 0.96 | 0.25 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3476 | 1/1   | 0.96 | 0.11 | 21,21,21,21                 | 0     |
| 86  | OHX  | c8    | 203  | 7/7   | 0.96 | 0.11 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3570 | 1/1   | 0.96 | 0.19 | 13,13,13,13                 | 0     |
| 85  | MG   | 5     | 3759 | 1/1   | 0.96 | 0.13 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3842 | 1/1   | 0.96 | 0.20 | 22,22,22,22                 | 0     |
| 86  | OHX  | 5     | 3949 | 7/7   | 0.96 | 0.14 | 84,84,84,84                 | 0     |
| 85  | MG   | 5     | 3415 | 1/1   | 0.96 | 0.20 | 19,19,19,19                 | 0     |
| 86  | OHX  | 5     | 3960 | 7/7   | 0.96 | 0.13 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 3963 | 7/7   | 0.96 | 0.13 | 77,77,77,77                 | 0     |
| 85  | MG   | 1     | 3725 | 1/1   | 0.96 | 0.05 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3512 | 1/1   | 0.96 | 0.29 | 22,22,22,22                 | 0     |
| 86  | OHX  | 5     | 3994 | 7/7   | 0.96 | 0.12 | 102,102,102,102             | 0     |
| 86  | OHX  | 3     | 219  | 7/7   | 0.96 | 0.11 | 96,96,96,96                 | 0     |
| 86  | OHX  | 3     | 220  | 7/7   | 0.96 | 0.11 | 101,101,101,101             | 0     |
| 85  | MG   | 5     | 3611 | 1/1   | 0.96 | 0.04 | 22,22,22,22                 | 0     |
| 86  | OHX  | 5     | 4013 | 7/7   | 0.96 | 0.10 | 129,129,129,129             | 0     |
| 85  | MG   | 5     | 3537 | 1/1   | 0.96 | 0.21 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3538 | 1/1   | 0.96 | 0.23 | 19,19,19,19                 | 0     |
| 86  | OHX  | 5     | 4022 | 7/7   | 0.96 | 0.14 | 87,87,87,87                 | 0     |
| 85  | MG   | SM    | 301  | 1/1   | 0.96 | 0.19 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4025 | 7/7   | 0.96 | 0.14 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3768 | 1/1   | 0.96 | 0.14 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3615 | 1/1   | 0.96 | 0.23 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 4089 | 7/7   | 0.96 | 0.09 | 159,159,159,159             | 0     |
| 85  | MG   | 5     | 3541 | 1/1   | 0.96 | 0.20 | 22,22,22,22                 | 0     |
| 86  | OHX  | 5     | 4031 | 7/7   | 0.96 | 0.12 | 110,110,110,110             | 0     |
| 86  | OHX  | 4     | 228  | 7/7   | 0.96 | 0.11 | 96,96,96,96                 | 0     |
| 85  | MG   | 2     | 1986 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3730 | 1/1   | 0.96 | 0.14 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3675 | 1/1   | 0.96 | 0.17 | 18,18,18,18                 | 0     |
| 85  | MG   | 2     | 1902 | 1/1   | 0.96 | 0.23 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4040 | 7/7   | 0.96 | 0.13 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3433 | 1/1   | 0.96 | 0.13 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3537 | 1/1   | 0.96 | 0.34 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3654 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4045 | 7/7   | 0.96 | 0.13 | 95,95,95,95                 | 0     |
| 86  | OHX  | 5     | 4046 | 7/7   | 0.96 | 0.21 | 78,78,78,78                 | 0     |
| 85  | MG   | 5     | 3624 | 1/1   | 0.96 | 0.14 | 18,18,18,18                 | 0     |
| 85  | MG   | 5     | 3426 | 1/1   | 0.96 | 0.25 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3626 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3705 | 1/1   | 0.96 | 0.15 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3628 | 1/1   | 0.96 | 0.15 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4054 | 7/7   | 0.96 | 0.14 | 86,86,86,86                 | 0     |
| 86  | OHX  | 5     | 4055 | 7/7   | 0.96 | 0.15 | 86,86,86,86                 | 0     |
| 85  | MG   | 1     | 3579 | 1/1   | 0.96 | 0.35 | 33,33,33,33                 | 0     |
| 86  | OHX  | M5    | 304  | 7/7   | 0.96 | 0.14 | 91,91,91,91                 | 0     |
| 86  | OHX  | 2     | 2038 | 7/7   | 0.96 | 0.14 | 97,97,97,97                 | 0     |
| 86  | OHX  | 5     | 4060 | 7/7   | 0.96 | 0.11 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3876 | 1/1   | 0.96 | 0.31 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3813 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 86  | OHX  | 2     | 2054 | 7/7   | 0.96 | 0.10 | 107,107,107,107             | 0     |
| 86  | OHX  | 2     | 2056 | 7/7   | 0.96 | 0.14 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 4065 | 7/7   | 0.96 | 0.12 | 91,91,91,91                 | 0     |
| 86  | OHX  | 2     | 2057 | 7/7   | 0.96 | 0.11 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4068 | 7/7   | 0.96 | 0.14 | 81,81,81,81                 | 0     |
| 86  | OHX  | 2     | 2066 | 7/7   | 0.96 | 0.15 | 89,89,89,89                 | 0     |
| 86  | OHX  | 5     | 4070 | 7/7   | 0.96 | 0.14 | 98,98,98,98                 | 0     |
| 86  | OHX  | 2     | 2067 | 7/7   | 0.96 | 0.11 | 114,114,114,114             | 0     |
| 86  | OHX  | 6     | 2086 | 7/7   | 0.96 | 0.12 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3580 | 1/1   | 0.96 | 0.24 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4074 | 7/7   | 0.96 | 0.14 | 93,93,93,93                 | 0     |
| 85  | MG   | 6     | 1943 | 1/1   | 0.96 | 0.29 | 32,32,32,32                 | 0     |
| 86  | OHX  | 2     | 2070 | 7/7   | 0.96 | 0.14 | 89,89,89,89                 | 0     |
| 86  | OHX  | 5     | 4077 | 7/7   | 0.96 | 0.09 | 136,136,136,136             | 0     |
| 86  | OHX  | 2     | 2074 | 7/7   | 0.96 | 0.10 | 111,111,111,111             | 0     |
| 86  | OHX  | 8     | 216  | 7/7   | 0.96 | 0.13 | 86,86,86,86                 | 0     |
| 86  | OHX  | 5     | 4080 | 7/7   | 0.96 | 0.12 | 95,95,95,95                 | 0     |
| 86  | OHX  | 5     | 4081 | 7/7   | 0.96 | 0.14 | 87,87,87,87                 | 0     |
| 86  | OHX  | 8     | 220  | 7/7   | 0.96 | 0.12 | 101,101,101,101             | 0     |
| 86  | OHX  | 6     | 2103 | 7/7   | 0.96 | 0.13 | 88,88,88,88                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86  | OHX  | SR    | 401  | 7/7   | 0.96 | 0.10 | 136,136,136,136            | 0     |
| 86  | OHX  | 6     | 2106 | 7/7   | 0.96 | 0.14 | 92,92,92,92                | 0     |
| 86  | OHX  | 1     | 3900 | 7/7   | 0.96 | 0.14 | 65,65,65,65                | 0     |
| 86  | OHX  | 6     | 2108 | 7/7   | 0.96 | 0.15 | 88,88,88,88                | 0     |
| 86  | OHX  | 6     | 2109 | 7/7   | 0.96 | 0.12 | 98,98,98,98                | 0     |
| 86  | OHX  | 2     | 2075 | 7/7   | 0.96 | 0.14 | 95,95,95,95                | 0     |
| 85  | MG   | 5     | 3788 | 1/1   | 0.96 | 0.07 | 39,39,39,39                | 0     |
| 86  | OHX  | l3    | 403  | 7/7   | 0.96 | 0.14 | 87,87,87,87                | 0     |
| 86  | OHX  | 6     | 2113 | 7/7   | 0.96 | 0.15 | 87,87,87,87                | 0     |
| 86  | OHX  | 2     | 2077 | 7/7   | 0.96 | 0.13 | 98,98,98,98                | 0     |
| 86  | OHX  | 5     | 4093 | 7/7   | 0.96 | 0.13 | 97,97,97,97                | 0     |
| 85  | MG   | 5     | 3882 | 1/1   | 0.96 | 0.18 | 19,19,19,19                | 0     |
| 86  | OHX  | 1     | 3944 | 7/7   | 0.96 | 0.12 | 87,87,87,87                | 0     |
| 86  | OHX  | 6     | 2118 | 7/7   | 0.96 | 0.16 | 89,89,89,89                | 0     |
| 86  | OHX  | 6     | 2119 | 7/7   | 0.96 | 0.12 | 107,107,107,107            | 0     |
| 86  | OHX  | 6     | 2121 | 7/7   | 0.96 | 0.15 | 89,89,89,89                | 0     |
| 86  | OHX  | 1     | 3950 | 7/7   | 0.96 | 0.13 | 89,89,89,89                | 0     |
| 85  | MG   | 1     | 3816 | 1/1   | 0.96 | 0.14 | 38,38,38,38                | 0     |
| 86  | OHX  | 1     | 3953 | 7/7   | 0.96 | 0.12 | 105,105,105,105            | 0     |
| 86  | OHX  | 1     | 3954 | 7/7   | 0.96 | 0.13 | 98,98,98,98                | 0     |
| 85  | MG   | 1     | 3682 | 1/1   | 0.96 | 0.23 | 50,50,50,50                | 0     |
| 86  | OHX  | o3    | 203  | 7/7   | 0.96 | 0.15 | 88,88,88,88                | 0     |
| 85  | MG   | 5     | 3557 | 1/1   | 0.96 | 0.20 | 21,21,21,21                | 0     |
| 85  | MG   | 5     | 3792 | 1/1   | 0.96 | 0.10 | 32,32,32,32                | 0     |
| 86  | OHX  | 2     | 2085 | 7/7   | 0.96 | 0.14 | 95,95,95,95                | 0     |
| 85  | MG   | 5     | 3793 | 1/1   | 0.96 | 0.05 | 36,36,36,36                | 0     |
| 87  | ZN   | e1    | 501  | 1/1   | 0.96 | 0.05 | 130,130,130,130            | 0     |
| 86  | OHX  | 1     | 3977 | 7/7   | 0.96 | 0.14 | 85,85,85,85                | 0     |
| 85  | MG   | 5     | 3558 | 1/1   | 0.96 | 0.23 | 24,24,24,24                | 0     |
| 86  | OHX  | 2     | 2088 | 7/7   | 0.96 | 0.13 | 101,101,101,101            | 0     |
| 85  | MG   | 1     | 3744 | 1/1   | 0.97 | 0.09 | 29,29,29,29                | 0     |
| 85  | MG   | 1     | 3728 | 1/1   | 0.97 | 0.15 | 27,27,27,27                | 0     |
| 85  | MG   | 1     | 3712 | 1/1   | 0.97 | 0.06 | 41,41,41,41                | 0     |
| 85  | MG   | 1     | 3550 | 1/1   | 0.97 | 0.25 | 31,31,31,31                | 0     |
| 85  | MG   | 1     | 3529 | 1/1   | 0.97 | 0.34 | 29,29,29,29                | 0     |
| 86  | OHX  | 2     | 2115 | 7/7   | 0.97 | 0.14 | 100,100,100,100            | 0     |
| 86  | OHX  | 1     | 3964 | 7/7   | 0.97 | 0.10 | 90,90,90,90                | 0     |
| 86  | OHX  | 1     | 3965 | 7/7   | 0.97 | 0.11 | 85,85,85,85                | 0     |
| 86  | OHX  | 1     | 3966 | 7/7   | 0.97 | 0.10 | 98,98,98,98                | 0     |
| 85  | MG   | 5     | 3682 | 1/1   | 0.97 | 0.05 | 22,22,22,22                | 0     |
| 85  | MG   | n8    | 204  | 1/1   | 0.97 | 0.19 | 25,25,25,25                | 0     |
| 86  | OHX  | 1     | 3971 | 7/7   | 0.97 | 0.16 | 75,75,75,75                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 3     | 217  | 7/7   | 0.97 | 0.13 | 86,86,86,86                 | 0     |
| 86  | OHX  | 3     | 218  | 7/7   | 0.97 | 0.15 | 81,81,81,81                 | 0     |
| 85  | MG   | 5     | 3584 | 1/1   | 0.97 | 0.30 | 19,19,19,19                 | 0     |
| 86  | OHX  | 1     | 3973 | 7/7   | 0.97 | 0.11 | 82,82,82,82                 | 0     |
| 86  | OHX  | 1     | 3974 | 7/7   | 0.97 | 0.10 | 86,86,86,86                 | 0     |
| 86  | OHX  | 1     | 3976 | 7/7   | 0.97 | 0.12 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3497 | 1/1   | 0.97 | 0.15 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 3978 | 7/7   | 0.97 | 0.10 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 3979 | 7/7   | 0.97 | 0.12 | 87,87,87,87                 | 0     |
| 86  | OHX  | 1     | 3980 | 7/7   | 0.97 | 0.13 | 87,87,87,87                 | 0     |
| 86  | OHX  | 4     | 224  | 7/7   | 0.97 | 0.10 | 93,93,93,93                 | 0     |
| 86  | OHX  | 4     | 225  | 7/7   | 0.97 | 0.12 | 97,97,97,97                 | 0     |
| 85  | MG   | 1     | 3786 | 1/1   | 0.97 | 0.19 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 3983 | 7/7   | 0.97 | 0.12 | 89,89,89,89                 | 0     |
| 85  | MG   | M7    | 206  | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 85  | MG   | 6     | 1995 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3496 | 1/1   | 0.97 | 0.19 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3637 | 1/1   | 0.97 | 0.12 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3502 | 1/1   | 0.97 | 0.26 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3639 | 1/1   | 0.97 | 0.17 | 40,40,40,40                 | 0     |
| 85  | MG   | 6     | 1997 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 86  | OHX  | 2     | 2031 | 7/7   | 0.97 | 0.14 | 80,80,80,80                 | 0     |
| 86  | OHX  | 2     | 2034 | 7/7   | 0.97 | 0.15 | 88,88,88,88                 | 0     |
| 86  | OHX  | 2     | 2036 | 7/7   | 0.97 | 0.11 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 3998 | 7/7   | 0.97 | 0.11 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 3999 | 7/7   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3743 | 1/1   | 0.97 | 0.23 | 22,22,22,22                 | 0     |
| 86  | OHX  | 5     | 3926 | 7/7   | 0.97 | 0.14 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 3940 | 7/7   | 0.97 | 0.13 | 69,69,69,69                 | 0     |
| 85  | MG   | 5     | 3797 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 3950 | 7/7   | 0.97 | 0.11 | 67,67,67,67                 | 0     |
| 86  | OHX  | 5     | 3951 | 7/7   | 0.97 | 0.16 | 95,95,95,95                 | 0     |
| 85  | MG   | 1     | 3811 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 3956 | 7/7   | 0.97 | 0.12 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 3958 | 7/7   | 0.97 | 0.12 | 71,71,71,71                 | 0     |
| 86  | OHX  | 2     | 2049 | 7/7   | 0.97 | 0.10 | 94,94,94,94                 | 0     |
| 86  | OHX  | 2     | 2050 | 7/7   | 0.97 | 0.10 | 95,95,95,95                 | 0     |
| 86  | OHX  | 2     | 2051 | 7/7   | 0.97 | 0.12 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 3975 | 7/7   | 0.97 | 0.12 | 75,75,75,75                 | 0     |
| 86  | OHX  | 2     | 2053 | 7/7   | 0.97 | 0.11 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 3981 | 7/7   | 0.97 | 0.16 | 71,71,71,71                 | 0     |
| 86  | OHX  | 5     | 3986 | 7/7   | 0.97 | 0.16 | 72,72,72,72                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 3988 | 7/7   | 0.97 | 0.10 | 97,97,97,97                 | 0     |
| 86  | OHX  | 5     | 3990 | 7/7   | 0.97 | 0.12 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 3992 | 7/7   | 0.97 | 0.11 | 81,81,81,81                 | 0     |
| 86  | OHX  | O7    | 103  | 7/7   | 0.97 | 0.13 | 77,77,77,77                 | 0     |
| 85  | MG   | 1     | 3812 | 1/1   | 0.97 | 0.10 | 27,27,27,27                 | 0     |
| 86  | OHX  | 5     | 3996 | 7/7   | 0.97 | 0.21 | 78,78,78,78                 | 0     |
| 86  | OHX  | 2     | 2055 | 7/7   | 0.97 | 0.10 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 4003 | 7/7   | 0.97 | 0.11 | 95,95,95,95                 | 0     |
| 86  | OHX  | 6     | 2066 | 7/7   | 0.97 | 0.15 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 4007 | 7/7   | 0.97 | 0.09 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 4011 | 7/7   | 0.97 | 0.12 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 4012 | 7/7   | 0.97 | 0.13 | 82,82,82,82                 | 0     |
| 86  | OHX  | 6     | 2071 | 7/7   | 0.97 | 0.09 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4015 | 7/7   | 0.97 | 0.12 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 4016 | 7/7   | 0.97 | 0.11 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3506 | 1/1   | 0.97 | 0.27 | 23,23,23,23                 | 0     |
| 86  | OHX  | 5     | 4018 | 7/7   | 0.97 | 0.11 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 4019 | 7/7   | 0.97 | 0.15 | 84,84,84,84                 | 0     |
| 86  | OHX  | 6     | 2078 | 7/7   | 0.97 | 0.16 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 4021 | 7/7   | 0.97 | 0.11 | 90,90,90,90                 | 0     |
| 86  | OHX  | 6     | 2084 | 7/7   | 0.97 | 0.11 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3518 | 1/1   | 0.97 | 0.27 | 19,19,19,19                 | 0     |
| 86  | OHX  | 2     | 2058 | 7/7   | 0.97 | 0.10 | 103,103,103,103             | 0     |
| 86  | OHX  | 6     | 2089 | 7/7   | 0.97 | 0.10 | 108,108,108,108             | 0     |
| 86  | OHX  | 2     | 2060 | 7/7   | 0.97 | 0.11 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4028 | 7/7   | 0.97 | 0.21 | 73,73,73,73                 | 0     |
| 86  | OHX  | 2     | 2061 | 7/7   | 0.97 | 0.14 | 84,84,84,84                 | 0     |
| 86  | OHX  | 6     | 2096 | 7/7   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 86  | OHX  | 6     | 2097 | 7/7   | 0.97 | 0.08 | 119,119,119,119             | 0     |
| 86  | OHX  | 2     | 2062 | 7/7   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 86  | OHX  | 6     | 2099 | 7/7   | 0.97 | 0.09 | 124,124,124,124             | 0     |
| 86  | OHX  | 2     | 2063 | 7/7   | 0.97 | 0.10 | 95,95,95,95                 | 0     |
| 86  | OHX  | 6     | 2101 | 7/7   | 0.97 | 0.10 | 134,134,134,134             | 0     |
| 86  | OHX  | 6     | 2102 | 7/7   | 0.97 | 0.09 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4038 | 7/7   | 0.97 | 0.09 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4039 | 7/7   | 0.97 | 0.28 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 4018 | 7/7   | 0.97 | 0.10 | 93,93,93,93                 | 0     |
| 86  | OHX  | 6     | 2104 | 7/7   | 0.97 | 0.10 | 100,100,100,100             | 0     |
| 86  | OHX  | 2     | 2064 | 7/7   | 0.97 | 0.10 | 104,104,104,104             | 0     |
| 86  | OHX  | 2     | 2065 | 7/7   | 0.97 | 0.12 | 87,87,87,87                 | 0     |
| 86  | OHX  | 5     | 4044 | 7/7   | 0.97 | 0.28 | 77,77,77,77                 | 0     |
| 85  | MG   | 1     | 3838 | 1/1   | 0.97 | 0.22 | 43,43,43,43                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3749 | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4047 | 7/7   | 0.97 | 0.11 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3646 | 1/1   | 0.97 | 0.19 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4049 | 7/7   | 0.97 | 0.15 | 83,83,83,83                 | 0     |
| 86  | OHX  | 6     | 2110 | 7/7   | 0.97 | 0.13 | 93,93,93,93                 | 0     |
| 85  | MG   | 5     | 3598 | 1/1   | 0.97 | 0.17 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3789 | 1/1   | 0.97 | 0.17 | 26,26,26,26                 | 0     |
| 86  | OHX  | 2     | 2071 | 7/7   | 0.97 | 0.09 | 108,108,108,108             | 0     |
| 86  | OHX  | 2     | 2072 | 7/7   | 0.97 | 0.12 | 100,100,100,100             | 0     |
| 86  | OHX  | 6     | 2115 | 7/7   | 0.97 | 0.11 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 4028 | 7/7   | 0.97 | 0.14 | 92,92,92,92                 | 0     |
| 86  | OHX  | 2     | 2073 | 7/7   | 0.97 | 0.11 | 95,95,95,95                 | 0     |
| 85  | MG   | 5     | 3434 | 1/1   | 0.97 | 0.18 | 24,24,24,24                 | 0     |
| 86  | OHX  | 5     | 4059 | 7/7   | 0.97 | 0.12 | 96,96,96,96                 | 0     |
| 85  | MG   | 5     | 3650 | 1/1   | 0.97 | 0.09 | 22,22,22,22                 | 0     |
| 86  | OHX  | 6     | 2120 | 7/7   | 0.97 | 0.11 | 93,93,93,93                 | 0     |
| 85  | MG   | 1     | 3661 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3402 | 1/1   | 0.97 | 0.13 | 16,16,16,16                 | 0     |
| 85  | MG   | 1     | 3404 | 1/1   | 0.97 | 0.33 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3753 | 1/1   | 0.97 | 0.13 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4036 | 7/7   | 0.97 | 0.12 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3405 | 1/1   | 0.97 | 0.15 | 18,18,18,18                 | 0     |
| 85  | MG   | 5     | 3606 | 1/1   | 0.97 | 0.24 | 18,18,18,18                 | 0     |
| 85  | MG   | 1     | 3498 | 1/1   | 0.97 | 0.20 | 20,20,20,20                 | 0     |
| 86  | OHX  | 2     | 2083 | 7/7   | 0.97 | 0.09 | 114,114,114,114             | 0     |
| 86  | OHX  | 6     | 2130 | 7/7   | 0.97 | 0.11 | 96,96,96,96                 | 0     |
| 86  | OHX  | 2     | 2084 | 7/7   | 0.97 | 0.11 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3561 | 1/1   | 0.97 | 0.38 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4043 | 7/7   | 0.97 | 0.13 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 4044 | 7/7   | 0.97 | 0.10 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 4217 | 1/1   | 0.97 | 0.19 | 19,19,19,19                 | 0     |
| 86  | OHX  | 1     | 4046 | 7/7   | 0.97 | 0.29 | 75,75,75,75                 | 0     |
| 85  | MG   | 5     | 3877 | 1/1   | 0.97 | 0.20 | 14,14,14,14                 | 0     |
| 86  | OHX  | 7     | 222  | 7/7   | 0.97 | 0.12 | 89,89,89,89                 | 0     |
| 86  | OHX  | 1     | 4048 | 7/7   | 0.97 | 0.12 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3442 | 1/1   | 0.97 | 0.16 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3583 | 1/1   | 0.97 | 0.26 | 31,31,31,31                 | 0     |
| 85  | MG   | 14    | 401  | 1/1   | 0.97 | 0.10 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4052 | 7/7   | 0.97 | 0.10 | 108,108,108,108             | 0     |
| 86  | OHX  | 2     | 2091 | 7/7   | 0.97 | 0.12 | 100,100,100,100             | 0     |
| 86  | OHX  | 8     | 217  | 7/7   | 0.97 | 0.10 | 102,102,102,102             | 0     |
| 85  | MG   | 5     | 3521 | 1/1   | 0.97 | 0.30 | 34,34,34,34                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 1901 | 1/1   | 0.97 | 0.23 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3411 | 1/1   | 0.97 | 0.18 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4090 | 7/7   | 0.97 | 0.24 | 79,79,79,79                 | 0     |
| 86  | OHX  | 8     | 222  | 7/7   | 0.97 | 0.10 | 114,114,114,114             | 0     |
| 86  | OHX  | 1     | 4175 | 7/7   | 0.97 | 0.14 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2095 | 7/7   | 0.97 | 0.07 | 132,132,132,132             | 0     |
| 85  | MG   | 5     | 3824 | 1/1   | 0.97 | 0.19 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3692 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4060 | 7/7   | 0.97 | 0.24 | 77,77,77,77                 | 0     |
| 85  | MG   | 5     | 3447 | 1/1   | 0.97 | 0.10 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3573 | 1/1   | 0.97 | 0.37 | 32,32,32,32                 | 0     |
| 86  | OHX  | C1    | 201  | 7/7   | 0.97 | 0.12 | 101,101,101,101             | 0     |
| 85  | MG   | m5    | 301  | 1/1   | 0.97 | 0.19 | 45,45,45,45                 | 0     |
| 85  | MG   | 6     | 1983 | 1/1   | 0.97 | 0.24 | 38,38,38,38                 | 0     |
| 86  | OHX  | C8    | 201  | 7/7   | 0.97 | 0.12 | 91,91,91,91                 | 0     |
| 86  | OHX  | 2     | 2102 | 7/7   | 0.97 | 0.10 | 110,110,110,110             | 0     |
| 86  | OHX  | 1     | 4068 | 7/7   | 0.97 | 0.26 | 78,78,78,78                 | 0     |
| 85  | MG   | 5     | 3829 | 1/1   | 0.97 | 0.14 | 59,59,59,59                 | 0     |
| 85  | MG   | 2     | 2022 | 1/1   | 0.97 | 0.07 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3909 | 7/7   | 0.97 | 0.10 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3446 | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 3916 | 7/7   | 0.97 | 0.10 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 3920 | 7/7   | 0.97 | 0.14 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 3921 | 7/7   | 0.97 | 0.11 | 79,79,79,79                 | 0     |
| 85  | MG   | 5     | 3453 | 1/1   | 0.97 | 0.30 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 3930 | 7/7   | 0.97 | 0.15 | 90,90,90,90                 | 0     |
| 85  | MG   | 1     | 3576 | 1/1   | 0.97 | 0.22 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 3937 | 7/7   | 0.97 | 0.10 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3577 | 1/1   | 0.97 | 0.24 | 23,23,23,23                 | 0     |
| 86  | OHX  | 1     | 3941 | 7/7   | 0.97 | 0.12 | 76,76,76,76                 | 0     |
| 86  | OHX  | 1     | 3942 | 7/7   | 0.97 | 0.15 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 3943 | 7/7   | 0.97 | 0.10 | 92,92,92,92                 | 0     |
| 85  | MG   | 1     | 3644 | 1/1   | 0.97 | 0.23 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 3948 | 7/7   | 0.97 | 0.10 | 90,90,90,90                 | 0     |
| 86  | OHX  | O7    | 104  | 7/7   | 0.98 | 0.17 | 75,75,75,75                 | 0     |
| 86  | OHX  | 1     | 3952 | 7/7   | 0.98 | 0.09 | 90,90,90,90                 | 0     |
| 86  | OHX  | Q2    | 503  | 7/7   | 0.98 | 0.18 | 64,64,64,64                 | 0     |
| 86  | OHX  | 6     | 2055 | 7/7   | 0.98 | 0.12 | 70,70,70,70                 | 0     |
| 86  | OHX  | 6     | 2059 | 7/7   | 0.98 | 0.13 | 81,81,81,81                 | 0     |
| 86  | OHX  | 5     | 4034 | 7/7   | 0.98 | 0.10 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3607 | 1/1   | 0.98 | 0.18 | 20,20,20,20                 | 0     |
| 86  | OHX  | 6     | 2065 | 7/7   | 0.98 | 0.09 | 78,78,78,78                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2039 | 7/7   | 0.98 | 0.10 | 83,83,83,83                 | 0     |
| 86  | OHX  | 6     | 2069 | 7/7   | 0.98 | 0.10 | 79,79,79,79                 | 0     |
| 86  | OHX  | 2     | 2040 | 7/7   | 0.98 | 0.11 | 79,79,79,79                 | 0     |
| 86  | OHX  | 6     | 2072 | 7/7   | 0.98 | 0.15 | 67,67,67,67                 | 0     |
| 86  | OHX  | 6     | 2073 | 7/7   | 0.98 | 0.09 | 99,99,99,99                 | 0     |
| 86  | OHX  | 6     | 2074 | 7/7   | 0.98 | 0.10 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3814 | 1/1   | 0.98 | 0.05 | 38,38,38,38                 | 0     |
| 86  | OHX  | 1     | 3958 | 7/7   | 0.98 | 0.14 | 75,75,75,75                 | 0     |
| 86  | OHX  | 6     | 2079 | 7/7   | 0.98 | 0.09 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2083 | 7/7   | 0.98 | 0.09 | 98,98,98,98                 | 0     |
| 86  | OHX  | 1     | 3959 | 7/7   | 0.98 | 0.13 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 3960 | 7/7   | 0.98 | 0.10 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 3961 | 7/7   | 0.98 | 0.16 | 72,72,72,72                 | 0     |
| 86  | OHX  | 6     | 2087 | 7/7   | 0.98 | 0.10 | 91,91,91,91                 | 0     |
| 86  | OHX  | 6     | 2088 | 7/7   | 0.98 | 0.08 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 3963 | 7/7   | 0.98 | 0.10 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2090 | 7/7   | 0.98 | 0.11 | 90,90,90,90                 | 0     |
| 85  | MG   | m6    | 201  | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 86  | OHX  | 6     | 2092 | 7/7   | 0.98 | 0.10 | 94,94,94,94                 | 0     |
| 86  | OHX  | 6     | 2093 | 7/7   | 0.98 | 0.10 | 87,87,87,87                 | 0     |
| 86  | OHX  | 6     | 2094 | 7/7   | 0.98 | 0.08 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2047 | 7/7   | 0.98 | 0.08 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3560 | 1/1   | 0.98 | 0.28 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3434 | 1/1   | 0.98 | 0.12 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 3968 | 7/7   | 0.98 | 0.18 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3969 | 7/7   | 0.98 | 0.13 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3539 | 1/1   | 0.98 | 0.26 | 19,19,19,19                 | 0     |
| 86  | OHX  | 5     | 4196 | 7/7   | 0.98 | 0.20 | 65,65,65,65                 | 0     |
| 86  | OHX  | 2     | 2052 | 7/7   | 0.98 | 0.09 | 83,83,83,83                 | 0     |
| 85  | MG   | M7    | 203  | 1/1   | 0.98 | 0.19 | 28,28,28,28                 | 0     |
| 86  | OHX  | 5     | 4066 | 7/7   | 0.98 | 0.10 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3519 | 1/1   | 0.98 | 0.22 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3860 | 1/1   | 0.98 | 0.08 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 3975 | 7/7   | 0.98 | 0.13 | 88,88,88,88                 | 0     |
| 85  | MG   | 6     | 1982 | 1/1   | 0.98 | 0.12 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3665 | 1/1   | 0.98 | 0.13 | 19,19,19,19                 | 0     |
| 85  | MG   | 5     | 3774 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 86  | OHX  | 2     | 2059 | 7/7   | 0.98 | 0.09 | 91,91,91,91                 | 0     |
| 85  | MG   | 5     | 3408 | 1/1   | 0.98 | 0.13 | 17,17,17,17                 | 0     |
| 85  | MG   | 1     | 3561 | 1/1   | 0.98 | 0.24 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 3982 | 7/7   | 0.98 | 0.27 | 69,69,69,69                 | 0     |
| 85  | MG   | L7    | 302  | 1/1   | 0.98 | 0.19 | 29,29,29,29                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4078 | 7/7   | 0.98 | 0.20 | 78,78,78,78                 | 0     |
| 85  | MG   | 1     | 4218 | 1/1   | 0.98 | 0.13 | 17,17,17,17                 | 0     |
| 86  | OHX  | 1     | 3985 | 7/7   | 0.98 | 0.19 | 69,69,69,69                 | 0     |
| 85  | MG   | M0    | 301  | 1/1   | 0.98 | 0.17 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 3988 | 7/7   | 0.98 | 0.19 | 73,73,73,73                 | 0     |
| 86  | OHX  | 1     | 3989 | 7/7   | 0.98 | 0.21 | 72,72,72,72                 | 0     |
| 85  | MG   | 5     | 3671 | 1/1   | 0.98 | 0.21 | 21,21,21,21                 | 0     |
| 86  | OHX  | 1     | 3894 | 7/7   | 0.98 | 0.13 | 64,64,64,64                 | 0     |
| 85  | MG   | 1     | 3422 | 1/1   | 0.98 | 0.13 | 23,23,23,23                 | 0     |
| 86  | OHX  | 5     | 3929 | 7/7   | 0.98 | 0.09 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 3931 | 7/7   | 0.98 | 0.10 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 3932 | 7/7   | 0.98 | 0.15 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3939 | 7/7   | 0.98 | 0.14 | 76,76,76,76                 | 0     |
| 86  | OHX  | 1     | 3901 | 7/7   | 0.98 | 0.12 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 3943 | 7/7   | 0.98 | 0.09 | 64,64,64,64                 | 0     |
| 86  | OHX  | 5     | 3944 | 7/7   | 0.98 | 0.11 | 71,71,71,71                 | 0     |
| 86  | OHX  | 5     | 3946 | 7/7   | 0.98 | 0.10 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 3947 | 7/7   | 0.98 | 0.09 | 72,72,72,72                 | 0     |
| 86  | OHX  | 3     | 215  | 7/7   | 0.98 | 0.10 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 3903 | 7/7   | 0.98 | 0.13 | 68,68,68,68                 | 0     |
| 86  | OHX  | 1     | 3904 | 7/7   | 0.98 | 0.11 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 3952 | 7/7   | 0.98 | 0.09 | 83,83,83,83                 | 0     |
| 85  | MG   | 1     | 3796 | 1/1   | 0.98 | 0.37 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 3912 | 7/7   | 0.98 | 0.10 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3913 | 7/7   | 0.98 | 0.11 | 72,72,72,72                 | 0     |
| 85  | MG   | 5     | 3597 | 1/1   | 0.98 | 0.12 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3803 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 3964 | 7/7   | 0.98 | 0.20 | 66,66,66,66                 | 0     |
| 86  | OHX  | 5     | 3965 | 7/7   | 0.98 | 0.10 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 3966 | 7/7   | 0.98 | 0.10 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 3967 | 7/7   | 0.98 | 0.12 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 3968 | 7/7   | 0.98 | 0.09 | 74,74,74,74                 | 0     |
| 86  | OHX  | 5     | 3969 | 7/7   | 0.98 | 0.09 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 3972 | 7/7   | 0.98 | 0.14 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3918 | 7/7   | 0.98 | 0.10 | 72,72,72,72                 | 0     |
| 86  | OHX  | 1     | 4002 | 7/7   | 0.98 | 0.08 | 115,115,115,115             | 0     |
| 86  | OHX  | 1     | 3919 | 7/7   | 0.98 | 0.10 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 3978 | 7/7   | 0.98 | 0.19 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 3979 | 7/7   | 0.98 | 0.11 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 3980 | 7/7   | 0.98 | 0.10 | 81,81,81,81                 | 0     |
| 86  | OHX  | 7     | 216  | 7/7   | 0.98 | 0.12 | 73,73,73,73                 | 0     |
| 86  | OHX  | 7     | 217  | 7/7   | 0.98 | 0.10 | 68,68,68,68                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 7     | 218  | 7/7   | 0.98 | 0.12 | 84,84,84,84                 | 0     |
| 86  | OHX  | 7     | 220  | 7/7   | 0.98 | 0.18 | 76,76,76,76                 | 0     |
| 86  | OHX  | 7     | 221  | 7/7   | 0.98 | 0.09 | 82,82,82,82                 | 0     |
| 86  | OHX  | 1     | 4004 | 7/7   | 0.98 | 0.21 | 72,72,72,72                 | 0     |
| 86  | OHX  | 5     | 3983 | 7/7   | 0.98 | 0.18 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3984 | 7/7   | 0.98 | 0.17 | 71,71,71,71                 | 0     |
| 86  | OHX  | 4     | 223  | 7/7   | 0.98 | 0.16 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3987 | 7/7   | 0.98 | 0.10 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3452 | 1/1   | 0.98 | 0.17 | 35,35,35,35                 | 0     |
| 86  | OHX  | 8     | 215  | 7/7   | 0.98 | 0.09 | 90,90,90,90                 | 0     |
| 85  | MG   | 3     | 210  | 1/1   | 0.98 | 0.22 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3720 | 1/1   | 0.98 | 0.22 | 42,42,42,42                 | 0     |
| 86  | OHX  | 5     | 3993 | 7/7   | 0.98 | 0.19 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3925 | 7/7   | 0.98 | 0.12 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3926 | 7/7   | 0.98 | 0.10 | 72,72,72,72                 | 0     |
| 86  | OHX  | 1     | 3928 | 7/7   | 0.98 | 0.09 | 72,72,72,72                 | 0     |
| 86  | OHX  | 5     | 3997 | 7/7   | 0.98 | 0.08 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 3998 | 7/7   | 0.98 | 0.08 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 4223 | 1/1   | 0.98 | 0.13 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 4000 | 7/7   | 0.98 | 0.09 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 4001 | 7/7   | 0.98 | 0.20 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 4002 | 7/7   | 0.98 | 0.19 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 4224 | 1/1   | 0.98 | 0.18 | 19,19,19,19                 | 0     |
| 86  | OHX  | 5     | 4004 | 7/7   | 0.98 | 0.13 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 4005 | 7/7   | 0.98 | 0.14 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3933 | 7/7   | 0.98 | 0.10 | 86,86,86,86                 | 0     |
| 86  | OHX  | 1     | 3934 | 7/7   | 0.98 | 0.12 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 4009 | 7/7   | 0.98 | 0.21 | 74,74,74,74                 | 0     |
| 86  | OHX  | 5     | 4010 | 7/7   | 0.98 | 0.10 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 3936 | 7/7   | 0.98 | 0.10 | 76,76,76,76                 | 0     |
| 85  | MG   | 5     | 3534 | 1/1   | 0.98 | 0.29 | 24,24,24,24                 | 0     |
| 86  | OHX  | 2     | 2026 | 7/7   | 0.98 | 0.15 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 4014 | 7/7   | 0.98 | 0.15 | 77,77,77,77                 | 0     |
| 86  | OHX  | 1     | 3940 | 7/7   | 0.98 | 0.09 | 80,80,80,80                 | 0     |
| 86  | OHX  | 2     | 2030 | 7/7   | 0.98 | 0.11 | 80,80,80,80                 | 0     |
| 85  | MG   | 1     | 3846 | 1/1   | 0.98 | 0.18 | 24,24,24,24                 | 0     |
| 86  | OHX  | m5    | 302  | 7/7   | 0.98 | 0.10 | 98,98,98,98                 | 0     |
| 86  | OHX  | m6    | 202  | 7/7   | 0.98 | 0.14 | 73,73,73,73                 | 0     |
| 86  | OHX  | 2     | 2032 | 7/7   | 0.98 | 0.09 | 89,89,89,89                 | 0     |
| 86  | OHX  | 2     | 2033 | 7/7   | 0.98 | 0.11 | 75,75,75,75                 | 0     |
| 86  | OHX  | o2    | 201  | 7/7   | 0.98 | 0.16 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 3945 | 7/7   | 0.98 | 0.09 | 82,82,82,82                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | M6    | 202  | 7/7   | 0.98 | 0.12 | 80,80,80,80                 | 0     |
| 86  | OHX  | o7    | 502  | 7/7   | 0.98 | 0.15 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3946 | 7/7   | 0.98 | 0.16 | 71,71,71,71                 | 0     |
| 87  | ZN   | E1    | 501  | 1/1   | 0.98 | 0.04 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3820 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 4024 | 7/7   | 0.98 | 0.09 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 3949 | 7/7   | 0.98 | 0.10 | 78,78,78,78                 | 0     |
| 86  | OHX  | O2    | 201  | 7/7   | 0.98 | 0.18 | 74,74,74,74                 | 0     |
| 86  | OHX  | 2     | 2035 | 7/7   | 0.98 | 0.13 | 82,82,82,82                 | 0     |
| 85  | MG   | 1     | 3599 | 1/1   | 0.98 | 0.31 | 20,20,20,20                 | 0     |
| 86  | OHX  | 5     | 3935 | 7/7   | 0.99 | 0.06 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 3936 | 7/7   | 0.99 | 0.07 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 3937 | 7/7   | 0.99 | 0.09 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 3938 | 7/7   | 0.99 | 0.10 | 71,71,71,71                 | 0     |
| 86  | OHX  | 6     | 2062 | 7/7   | 0.99 | 0.08 | 71,71,71,71                 | 0     |
| 86  | OHX  | 6     | 2063 | 7/7   | 0.99 | 0.07 | 71,71,71,71                 | 0     |
| 86  | OHX  | 5     | 3941 | 7/7   | 0.99 | 0.08 | 67,67,67,67                 | 0     |
| 86  | OHX  | 5     | 3942 | 7/7   | 0.99 | 0.09 | 75,75,75,75                 | 0     |
| 86  | OHX  | 2     | 2027 | 7/7   | 0.99 | 0.09 | 69,69,69,69                 | 0     |
| 86  | OHX  | 2     | 2045 | 7/7   | 0.99 | 0.08 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 3945 | 7/7   | 0.99 | 0.08 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 3927 | 7/7   | 0.99 | 0.09 | 56,56,56,56                 | 0     |
| 86  | OHX  | 6     | 2067 | 7/7   | 0.99 | 0.15 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 3948 | 7/7   | 0.99 | 0.07 | 85,85,85,85                 | 0     |
| 86  | OHX  | 6     | 2068 | 7/7   | 0.99 | 0.13 | 71,71,71,71                 | 0     |
| 86  | OHX  | 2     | 2046 | 7/7   | 0.99 | 0.06 | 86,86,86,86                 | 0     |
| 86  | OHX  | 6     | 2070 | 7/7   | 0.99 | 0.12 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3929 | 7/7   | 0.99 | 0.16 | 63,63,63,63                 | 0     |
| 86  | OHX  | 5     | 3954 | 7/7   | 0.99 | 0.08 | 74,74,74,74                 | 0     |
| 86  | OHX  | 2     | 2028 | 7/7   | 0.99 | 0.06 | 62,62,62,62                 | 0     |
| 86  | OHX  | 1     | 3986 | 7/7   | 0.99 | 0.08 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 3957 | 7/7   | 0.99 | 0.08 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3931 | 7/7   | 0.99 | 0.09 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 3959 | 7/7   | 0.99 | 0.08 | 58,58,58,58                 | 0     |
| 86  | OHX  | 6     | 2075 | 7/7   | 0.99 | 0.12 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 3961 | 7/7   | 0.99 | 0.09 | 72,72,72,72                 | 0     |
| 86  | OHX  | 5     | 3962 | 7/7   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 86  | OHX  | 6     | 2076 | 7/7   | 0.99 | 0.08 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2048 | 7/7   | 0.99 | 0.05 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 3872 | 7/7   | 0.99 | 0.15 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 3874 | 7/7   | 0.99 | 0.12 | 48,48,48,48                 | 0     |
| 86  | OHX  | 6     | 2080 | 7/7   | 0.99 | 0.13 | 79,79,79,79                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 6     | 2081 | 7/7   | 0.99 | 0.11 | 78,78,78,78                 | 0     |
| 86  | OHX  | 6     | 2082 | 7/7   | 0.99 | 0.07 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 3970 | 7/7   | 0.99 | 0.06 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3971 | 7/7   | 0.99 | 0.11 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3935 | 7/7   | 0.99 | 0.08 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 3973 | 7/7   | 0.99 | 0.08 | 62,62,62,62                 | 0     |
| 86  | OHX  | 1     | 3877 | 7/7   | 0.99 | 0.10 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 3878 | 7/7   | 0.99 | 0.12 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 3976 | 7/7   | 0.99 | 0.08 | 85,85,85,85                 | 0     |
| 86  | OHX  | 1     | 3938 | 7/7   | 0.99 | 0.09 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 3879 | 7/7   | 0.99 | 0.08 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 3880 | 7/7   | 0.99 | 0.08 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 3882 | 7/7   | 0.99 | 0.08 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 3883 | 7/7   | 0.99 | 0.12 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 3982 | 7/7   | 0.99 | 0.13 | 63,63,63,63                 | 0     |
| 86  | OHX  | 1     | 3885 | 7/7   | 0.99 | 0.09 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 3886 | 7/7   | 0.99 | 0.10 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 3985 | 7/7   | 0.99 | 0.13 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 3889 | 7/7   | 0.99 | 0.09 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 3891 | 7/7   | 0.99 | 0.12 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3947 | 7/7   | 0.99 | 0.17 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 3989 | 7/7   | 0.99 | 0.09 | 62,62,62,62                 | 0     |
| 86  | OHX  | 1     | 3893 | 7/7   | 0.99 | 0.07 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 3991 | 7/7   | 0.99 | 0.13 | 69,69,69,69                 | 0     |
| 86  | OHX  | 2     | 2029 | 7/7   | 0.99 | 0.09 | 75,75,75,75                 | 0     |
| 86  | OHX  | 1     | 3895 | 7/7   | 0.99 | 0.07 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 3897 | 7/7   | 0.99 | 0.09 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 3898 | 7/7   | 0.99 | 0.09 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3562 | 1/1   | 0.99 | 0.30 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3662 | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 86  | OHX  | 1     | 3955 | 7/7   | 0.99 | 0.09 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3902 | 7/7   | 0.99 | 0.08 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3500 | 1/1   | 0.99 | 0.34 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3829 | 1/1   | 0.99 | 0.07 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 3905 | 7/7   | 0.99 | 0.09 | 52,52,52,52                 | 0     |
| 86  | OHX  | 1     | 3906 | 7/7   | 0.99 | 0.06 | 57,57,57,57                 | 0     |
| 86  | OHX  | 1     | 3907 | 7/7   | 0.99 | 0.07 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 3962 | 7/7   | 0.99 | 0.16 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 3908 | 7/7   | 0.99 | 0.05 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3804 | 1/1   | 0.99 | 0.08 | 45,45,45,45                 | 0     |
| 86  | OHX  | 7     | 219  | 7/7   | 0.99 | 0.14 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 4008 | 7/7   | 0.99 | 0.14 | 64,64,64,64                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3910 | 7/7   | 0.99 | 0.08 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3911 | 7/7   | 0.99 | 0.08 | 70,70,70,70                 | 0     |
| 86  | OHX  | M5    | 303  | 7/7   | 0.99 | 0.07 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3772 | 1/1   | 0.99 | 0.10 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3473 | 1/1   | 0.99 | 0.22 | 18,18,18,18                 | 0     |
| 86  | OHX  | 1     | 3914 | 7/7   | 0.99 | 0.06 | 58,58,58,58                 | 0     |
| 86  | OHX  | 2     | 2037 | 7/7   | 0.99 | 0.09 | 71,71,71,71                 | 0     |
| 86  | OHX  | 8     | 214  | 7/7   | 0.99 | 0.09 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3835 | 1/1   | 0.99 | 0.06 | 46,46,46,46                 | 0     |
| 86  | OHX  | N9    | 101  | 7/7   | 0.99 | 0.11 | 48,48,48,48                 | 0     |
| 86  | OHX  | 1     | 3917 | 7/7   | 0.99 | 0.09 | 70,70,70,70                 | 0     |
| 86  | OHX  | 2     | 2024 | 7/7   | 0.99 | 0.11 | 62,62,62,62                 | 0     |
| 86  | OHX  | 2     | 2025 | 7/7   | 0.99 | 0.10 | 66,66,66,66                 | 0     |
| 85  | MG   | 5     | 3836 | 1/1   | 0.99 | 0.09 | 22,22,22,22                 | 0     |
| 86  | OHX  | s1    | 302  | 7/7   | 0.99 | 0.14 | 67,67,67,67                 | 0     |
| 86  | OHX  | 2     | 2042 | 7/7   | 0.99 | 0.09 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 3922 | 7/7   | 0.99 | 0.08 | 77,77,77,77                 | 0     |
| 86  | OHX  | 6     | 2048 | 7/7   | 0.99 | 0.13 | 60,60,60,60                 | 0     |
| 86  | OHX  | 6     | 2049 | 7/7   | 0.99 | 0.09 | 51,51,51,51                 | 0     |
| 86  | OHX  | 6     | 2050 | 7/7   | 0.99 | 0.10 | 60,60,60,60                 | 0     |
| 86  | OHX  | 6     | 2051 | 7/7   | 0.99 | 0.11 | 60,60,60,60                 | 0     |
| 86  | OHX  | 6     | 2053 | 7/7   | 0.99 | 0.11 | 61,61,61,61                 | 0     |
| 86  | OHX  | 6     | 2054 | 7/7   | 0.99 | 0.10 | 69,69,69,69                 | 0     |
| 86  | OHX  | l3    | 402  | 7/7   | 0.99 | 0.11 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 3923 | 7/7   | 0.99 | 0.07 | 69,69,69,69                 | 0     |
| 86  | OHX  | 6     | 2056 | 7/7   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 86  | OHX  | 6     | 2057 | 7/7   | 0.99 | 0.07 | 63,63,63,63                 | 0     |
| 86  | OHX  | 5     | 3898 | 7/7   | 0.99 | 0.12 | 37,37,37,37                 | 0     |
| 86  | OHX  | 5     | 3902 | 7/7   | 0.99 | 0.14 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 3904 | 7/7   | 0.99 | 0.09 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 3905 | 7/7   | 0.99 | 0.09 | 45,45,45,45                 | 0     |
| 86  | OHX  | 5     | 3906 | 7/7   | 0.99 | 0.09 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 3907 | 7/7   | 0.99 | 0.11 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 3909 | 7/7   | 0.99 | 0.14 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 3910 | 7/7   | 0.99 | 0.08 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 3912 | 7/7   | 0.99 | 0.10 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 3913 | 7/7   | 0.99 | 0.10 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 3914 | 7/7   | 0.99 | 0.11 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 3916 | 7/7   | 0.99 | 0.07 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 3918 | 7/7   | 0.99 | 0.08 | 56,56,56,56                 | 0     |
| 86  | OHX  | n3    | 203  | 7/7   | 0.99 | 0.09 | 69,69,69,69                 | 0     |
| 86  | OHX  | n9    | 3803 | 7/7   | 0.99 | 0.10 | 52,52,52,52                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 3920 | 7/7   | 0.99 | 0.07 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 3921 | 7/7   | 0.99 | 0.09 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 3922 | 7/7   | 0.99 | 0.09 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 3923 | 7/7   | 0.99 | 0.10 | 57,57,57,57                 | 0     |
| 86  | OHX  | q2    | 502  | 7/7   | 0.99 | 0.16 | 67,67,67,67                 | 0     |
| 86  | OHX  | 5     | 3924 | 7/7   | 0.99 | 0.07 | 52,52,52,52                 | 0     |
| 86  | OHX  | 6     | 2058 | 7/7   | 0.99 | 0.08 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 3927 | 7/7   | 0.99 | 0.06 | 59,59,59,59                 | 0     |
| 87  | ZN   | Q3    | 501  | 1/1   | 0.99 | 0.02 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 3928 | 7/7   | 0.99 | 0.06 | 55,55,55,55                 | 0     |
| 86  | OHX  | 2     | 2043 | 7/7   | 0.99 | 0.07 | 80,80,80,80                 | 0     |
| 86  | OHX  | 6     | 2060 | 7/7   | 0.99 | 0.06 | 69,69,69,69                 | 0     |
| 86  | OHX  | 6     | 2061 | 7/7   | 0.99 | 0.07 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 3933 | 7/7   | 0.99 | 0.07 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 3896 | 7/7   | 1.00 | 0.04 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 3911 | 7/7   | 1.00 | 0.06 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 3875 | 7/7   | 1.00 | 0.06 | 41,41,41,41                 | 0     |
| 86  | OHX  | 4     | 222  | 7/7   | 1.00 | 0.09 | 46,46,46,46                 | 0     |
| 86  | OHX  | 6     | 2047 | 7/7   | 1.00 | 0.10 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 3915 | 7/7   | 1.00 | 0.07 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 3884 | 7/7   | 1.00 | 0.05 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 3917 | 7/7   | 1.00 | 0.06 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 3899 | 7/7   | 1.00 | 0.06 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 3919 | 7/7   | 1.00 | 0.07 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 3876 | 7/7   | 1.00 | 0.10 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 3870 | 7/7   | 1.00 | 0.10 | 35,35,35,35                 | 0     |
| 86  | OHX  | 6     | 2052 | 7/7   | 1.00 | 0.07 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 3953 | 7/7   | 1.00 | 0.06 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 3887 | 7/7   | 1.00 | 0.05 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 3888 | 7/7   | 1.00 | 0.08 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 3925 | 7/7   | 1.00 | 0.04 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 3871 | 7/7   | 1.00 | 0.12 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 3899 | 7/7   | 1.00 | 0.11 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 3900 | 7/7   | 1.00 | 0.11 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 3901 | 7/7   | 1.00 | 0.10 | 37,37,37,37                 | 0     |
| 86  | OHX  | 5     | 3930 | 7/7   | 1.00 | 0.04 | 48,48,48,48                 | 0     |
| 87  | ZN   | D6    | 500  | 1/1   | 1.00 | 0.01 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3890 | 7/7   | 1.00 | 0.06 | 53,53,53,53                 | 0     |
| 87  | ZN   | D9    | 101  | 1/1   | 1.00 | 0.02 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 3903 | 7/7   | 1.00 | 0.11 | 43,43,43,43                 | 0     |
| 87  | ZN   | O7    | 101  | 1/1   | 1.00 | 0.01 | 25,25,25,25                 | 0     |
| 87  | ZN   | Q0    | 500  | 1/1   | 1.00 | 0.02 | 35,35,35,35                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3868 | 7/7   | 1.00 | 0.11 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 3934 | 7/7   | 1.00 | 0.06 | 62,62,62,62                 | 0     |
| 87  | ZN   | d6    | 101  | 1/1   | 1.00 | 0.01 | 48,48,48,48                 | 0     |
| 86  | OHX  | 1     | 3892 | 7/7   | 1.00 | 0.05 | 56,56,56,56                 | 0     |
| 87  | ZN   | d9    | 101  | 1/1   | 1.00 | 0.02 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 3873 | 7/7   | 1.00 | 0.08 | 42,42,42,42                 | 0     |
| 87  | ZN   | o7    | 501  | 1/1   | 1.00 | 0.01 | 29,29,29,29                 | 0     |
| 87  | ZN   | q0    | 201  | 1/1   | 1.00 | 0.02 | 23,23,23,23                 | 0     |
| 86  | OHX  | 1     | 3881 | 7/7   | 1.00 | 0.04 | 46,46,46,46                 | 0     |
| 87  | ZN   | q3    | 501  | 1/1   | 1.00 | 0.02 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 3908 | 7/7   | 1.00 | 0.06 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 3869 | 7/7   | 1.00 | 0.09 | 38,38,38,38                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.