



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:41 pm BST

PDB ID : 4P6F  
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome  
Authors : Fagan, C.E.; Dunham, C.M.  
Deposited on : 2014-03-24  
Resolution : 3.60 Å(reported)

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

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

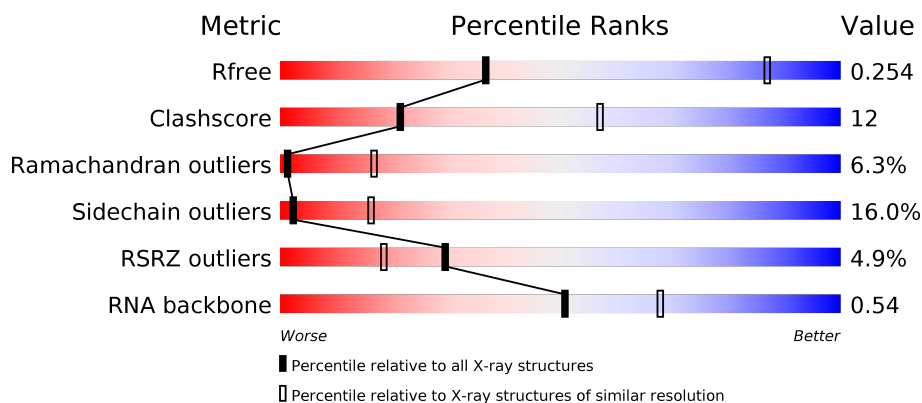
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1257 (3.70-3.50)                                      |
| Clashscore            | 141614                      | 1353 (3.70-3.50)                                      |
| Ramachandran outliers | 138981                      | 1307 (3.70-3.50)                                      |
| Sidechain outliers    | 138945                      | 1307 (3.70-3.50)                                      |
| RSRZ outliers         | 127900                      | 1161 (3.70-3.50)                                      |
| RNA backbone          | 3102                        | 1017 (4.20-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | QA    | 1522   | <div> <div>4%</div> <div>54%</div> <div>35%</div> <div>9%</div> <div>..</div> </div>  |
| 1   | XA    | 1522   | <div> <div>3%</div> <div>56%</div> <div>33%</div> <div>9%</div> <div>.</div> </div>   |
| 2   | QB    | 256    | <div> <div>10%</div> <div>48%</div> <div>36%</div> <div>7%</div> <div>7%</div> </div> |
| 2   | XB    | 256    | <div> <div>5%</div> <div>46%</div> <div>36%</div> <div>10%</div> <div>7%</div> </div> |

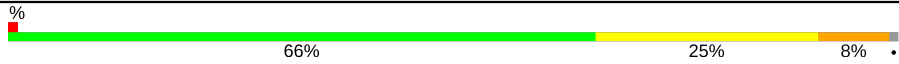
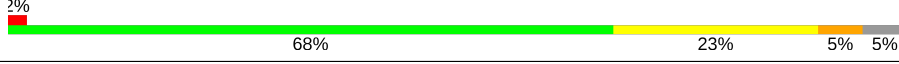




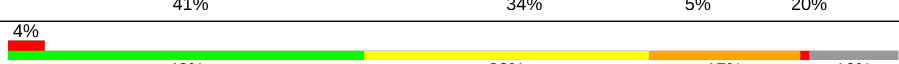
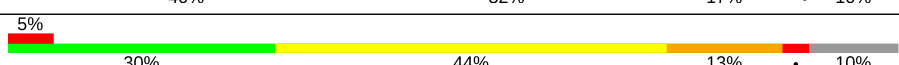
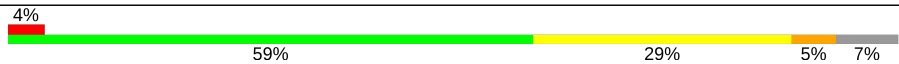


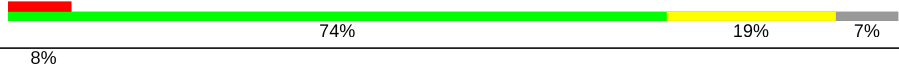




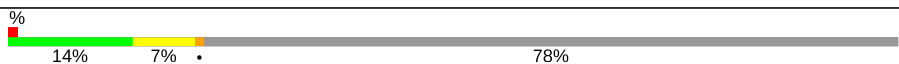








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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | QC    | 239    |                  |
| 3   | XC    | 239    |                  |
| 4   | QD    | 209    |                  |
| 4   | XD    | 209    |   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





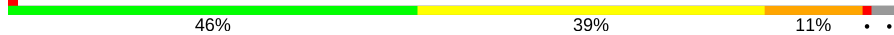




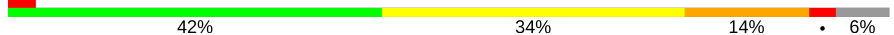
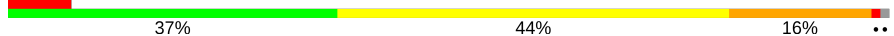
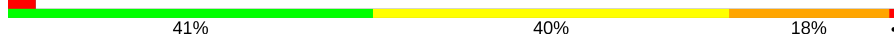













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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | XO    | 89     |    |
| 16  | QP    | 88     |    |
| 16  | XP    | 88     |    |
| 17  | QQ    | 105    |    |
| 17  | XQ    | 105    |    |
| 18  | QR    | 88     |    |
| 18  | XR    | 88     |    |
| 19  | QS    | 93     |    |
| 19  | XS    | 93     |    |
| 20  | QT    | 106    |    |
| 20  | XT    | 106    |   |
| 21  | QU    | 27     |  |
| 21  | XU    | 27     |  |
| 22  | QV    | 77     |  |
| 22  | XV    | 77     |  |
| 23  | QW    | 76     |  |
| 23  | QY    | 76     |  |
| 23  | XW    | 76     |  |
| 23  | XY    | 76     |  |
| 24  | QX    | 24     |  |
| 24  | XX    | 24     |  |
| 25  | RA    | 2915   |  |
| 25  | YA    | 2915   |  |
| 26  | RB    | 122    |  |
| 26  | YB    | 122    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 27  | RD    | 276    |    |
| 27  | YD    | 276    |    |
| 28  | RE    | 206    |    |
| 28  | YE    | 206    |    |
| 29  | RF    | 210    |    |
| 29  | YF    | 210    |    |
| 30  | RG    | 182    |    |
| 30  | YG    | 182    |    |
| 31  | RH    | 180    |    |
| 31  | YH    | 180    |    |
| 32  | RI    | 148    |    |
| 32  | YI    | 148    |   |
| 33  | RN    | 140    |  |
| 33  | YN    | 140    |  |
| 34  | RO    | 122    |  |
| 34  | YO    | 122    |  |
| 35  | RP    | 150    |  |
| 35  | YP    | 150    |  |
| 36  | RQ    | 141    |  |
| 36  | YQ    | 141    |  |
| 37  | RR    | 118    |  |
| 37  | YR    | 118    |  |
| 38  | RS    | 112    |  |
| 38  | YS    | 112    |  |
| 39  | RT    | 146    |  |

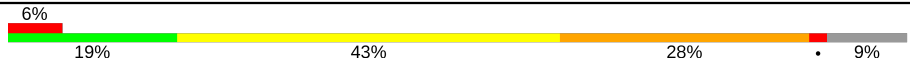
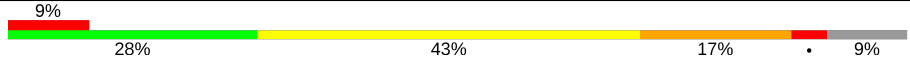



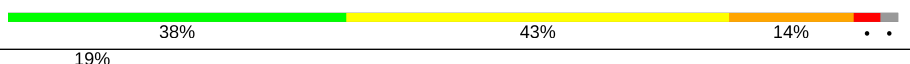



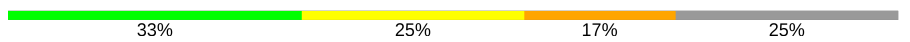
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | YT    | 146    |                  |
| 40  | RU    | 118    |                  |
| 40  | YU    | 118    |                  |
| 41  | RV    | 101    |                  |
| 41  | YV    | 101    |                  |
| 42  | RW    | 113    |                  |
| 42  | YW    | 113    |                  |
| 43  | RX    | 96     |                  |
| 43  | YX    | 96     |                  |
| 44  | RY    | 110    |                  |
| 44  | YY    | 110    |                  |
| 45  | RZ    | 206    |                  |
| 45  | YZ    | 206    |                  |
| 46  | R0    | 85     |                  |
| 46  | Y0    | 85     |                  |
| 47  | R1    | 98     |                  |
| 47  | Y1    | 98     |                  |
| 48  | R2    | 72     |                  |
| 48  | Y2    | 72     |                  |
| 49  | R3    | 60     |                  |
| 49  | Y3    | 60     |                  |
| 50  | R4    | 71     |                  |
| 50  | Y4    | 71     |                  |
| 51  | R5    | 60     |                  |
| 51  | Y5    | 60     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 52  | R6    | 54     |  |
| 52  | Y6    | 54     |  |
| 53  | R7    | 49     |  |
| 53  | Y7    | 49     |  |
| 54  | R8    | 65     |  |
| 54  | Y8    | 65     |  |
| 55  | R9    | 37     |  |
| 55  | Y9    | 37     |  |
| 56  | Z7    | 12     |  |
| 56  | Z8    | 12     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | QA    | 1603 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1638 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1644 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1649 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1655 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1664 | -         | -        | -       | X                |
| 57  | MG   | R0    | 101  | -         | -        | -       | X                |
| 57  | MG   | R5    | 101  | -         | -        | -       | X                |
| 57  | MG   | RA    | 3002 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3007 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3044 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3118 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3127 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3132 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3138 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3153 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3157 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3159 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3161 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3164 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | RA    | 3171 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3175 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3185 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3196 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3197 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3201 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3203 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3206 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3212 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3216 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3217 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3218 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3219 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3220 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3224 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3225 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3238 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3239 | -         | -        | -       | X                |
| 57  | MG   | RD    | 301  | -         | -        | -       | X                |
| 57  | MG   | RP    | 204  | -         | -        | -       | X                |
| 57  | MG   | XA    | 1601 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1608 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1609 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1634 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1650 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1662 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1670 | -         | -        | -       | X                |
| 57  | MG   | XB    | 301  | -         | -        | -       | X                |
| 57  | MG   | XM    | 201  | -         | -        | -       | X                |
| 57  | MG   | YA    | 3012 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3054 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3125 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3149 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3153 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3156 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3161 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3178 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3190 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3201 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3210 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3214 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3228 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | YA    | 3231 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3233 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3243 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3254 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3258 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3259 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3274 | -         | -        | -       | X                |
| 57  | MG   | YB    | 201  | -         | -        | -       | X                |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called E-Site tRNA-Phe or A-Site tRNA-Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | QW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1619  | 723 | 290 | 531 | 75 |         |         |       |
| 23  | QY    | 17       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 364   | 163 | 68  | 116 | 17 |         |         |       |
| 23  | XW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1619  | 723 | 290 | 531 | 75 |         |         |       |
| 23  | XY    | 17       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 364   | 163 | 68  | 116 | 17 |         |         |       |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 24  | QX    | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 210   | 96 | 39 | 66 | 9 |         |         |       |
| 24  | XX    | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 210   | 96 | 39 | 66 | 9 |         |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25  | RA    | 2882     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62071 | 27627 | 11611 | 19952 | 2881 |         |         |       |
| 25  | YA    | 2883     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62091 | 27636 | 11613 | 19960 | 2882 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | R5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 51  | Y5    | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 278 | 88 | 71 | 5 |         |         |       |

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

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

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

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

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

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

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

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

- Molecule 56 is a protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 56  | Z7    | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 116   | 78 | 18 | 20 |         |         |       |
| 56  | Z8    | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 116   | 78 | 18 | 20 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | QA    | 67       | Total | Mg  | 0       | 0       |
|     |       |          | 67    | 67  |         |         |
| 57  | RP    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 57  | YA    | 278      | Total | Mg  | 0       | 0       |
|     |       |          | 278   | 278 |         |         |
| 57  | Y5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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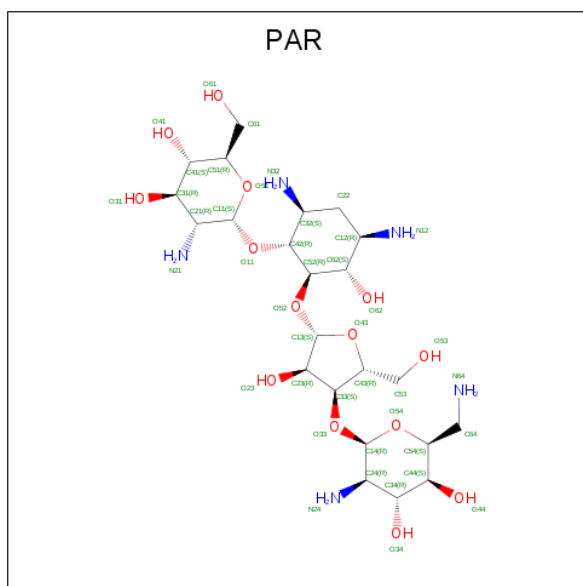
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | YD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | QV    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | XA    | 71       | Total<br>71  | Mg<br>71  | 0       | 0       |
| 57  | R0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | QH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | YX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | Y7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XB    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | QF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | R5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RA    | 246      | Total<br>246 | Mg<br>246 | 0       | 0       |
| 57  | YP    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | YB    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | QY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XV    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | RB    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | XM    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | YE    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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

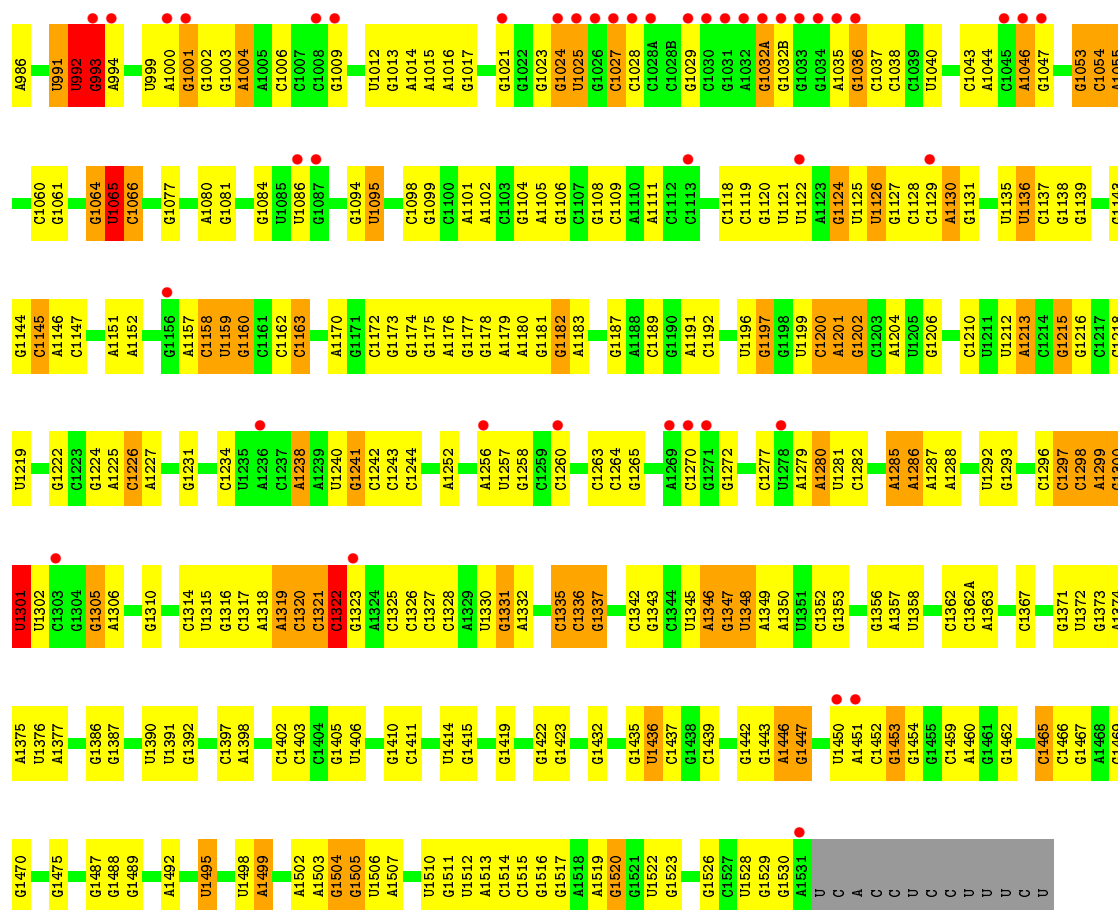


| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 58  | QA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |
| 58  | XA    | 1       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

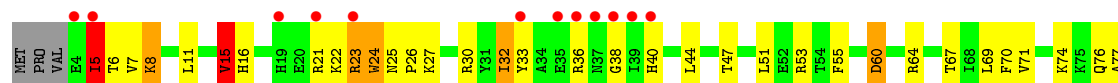
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

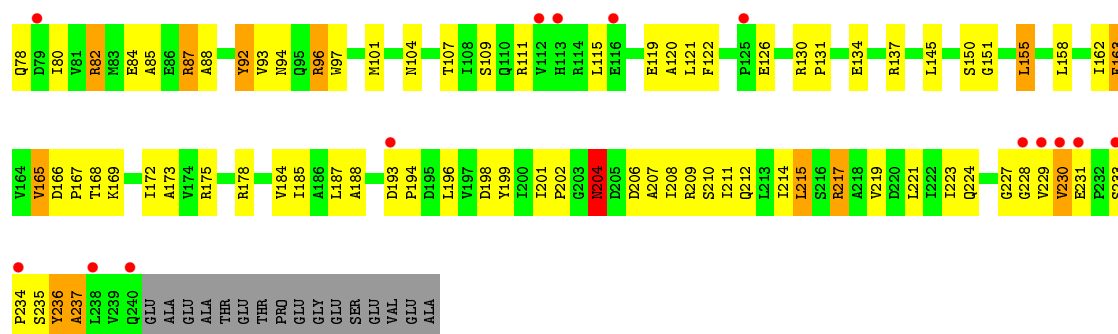
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | Y9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | QN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | R5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | QD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |



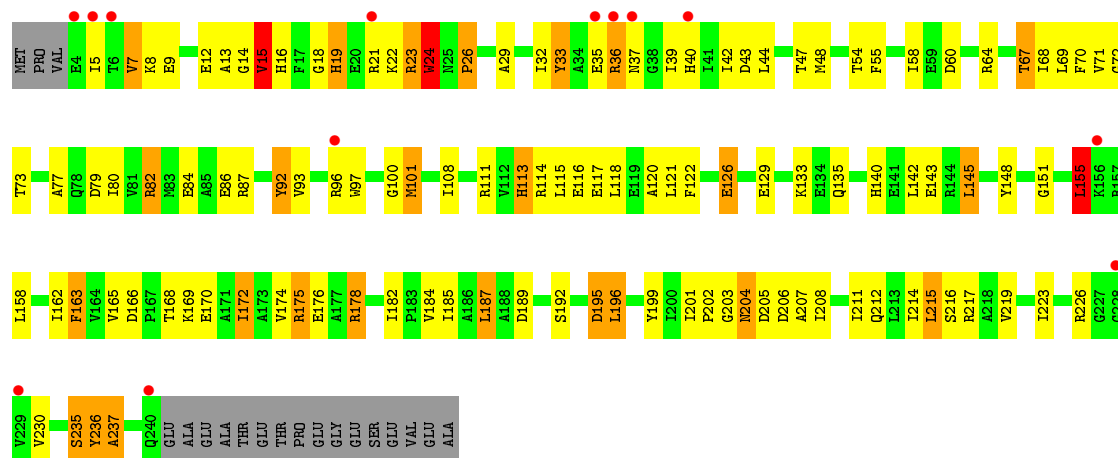




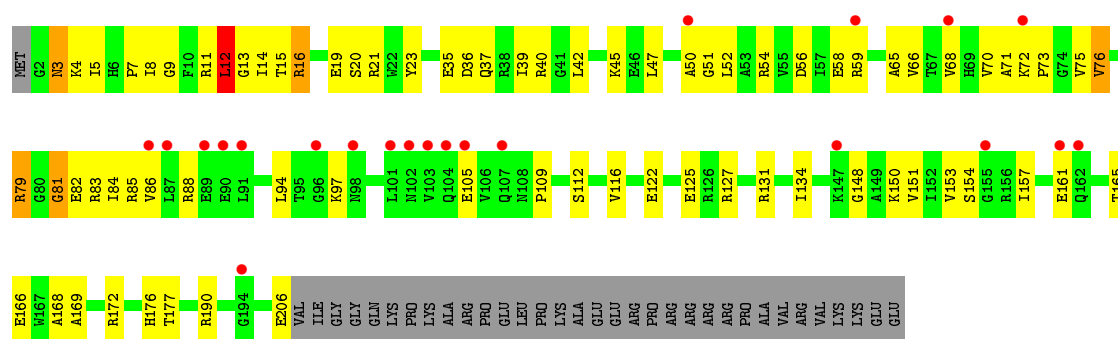




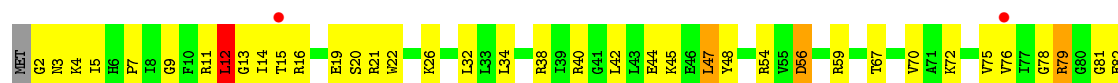
• Molecule 2: 30S ribosomal protein S2

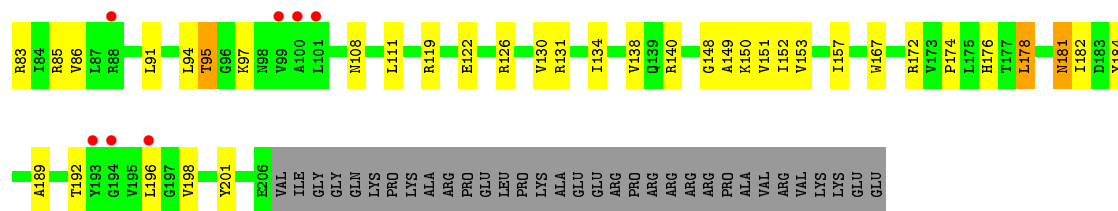


• Molecule 3: 30S ribosomal protein S3

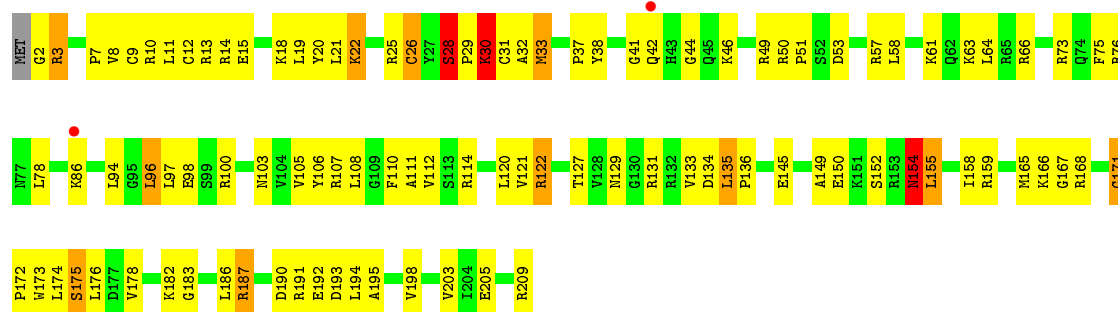


• Molecule 3: 30S ribosomal protein S3

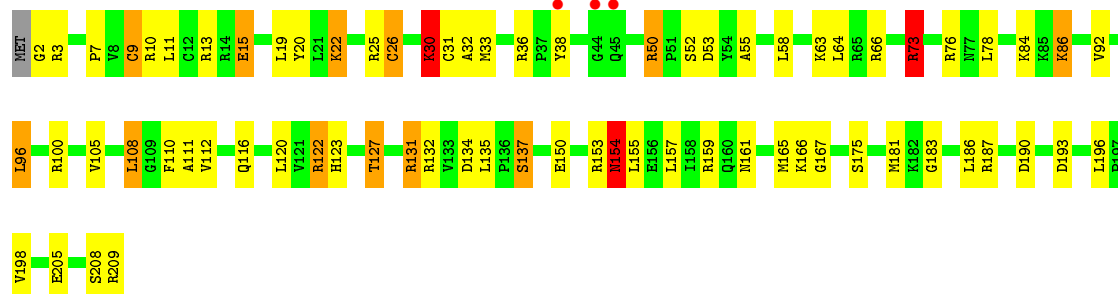




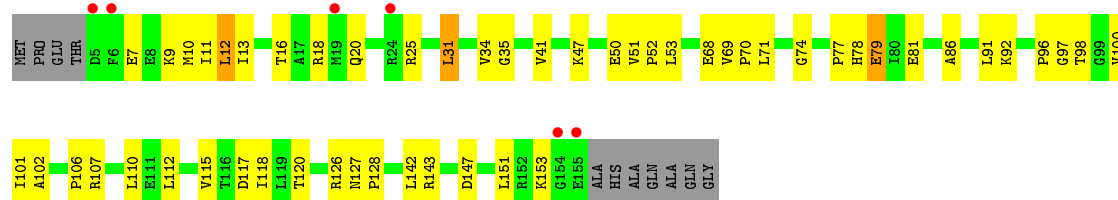
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

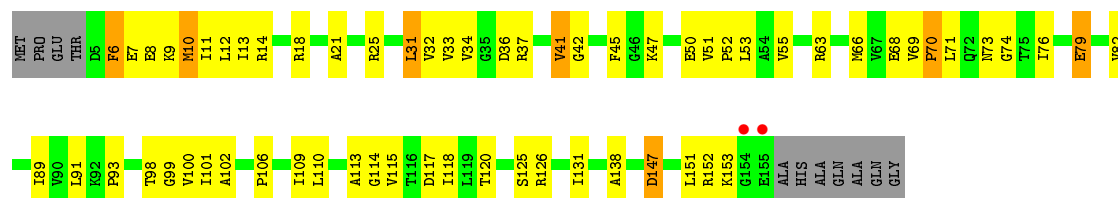


• Molecule 5: 30S ribosomal protein S5

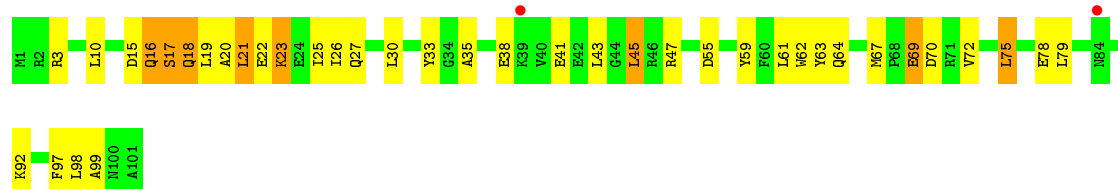


• Molecule 5: 30S ribosomal protein S5





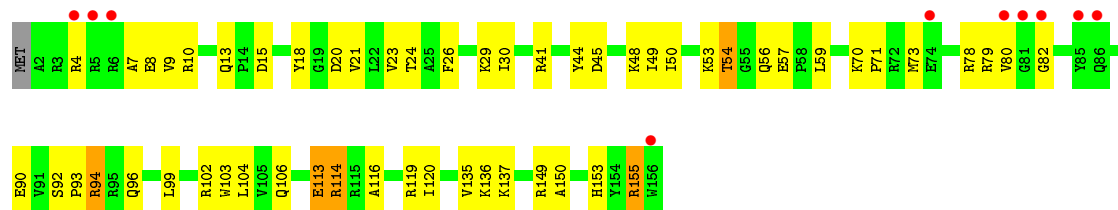
• Molecule 6: 30S ribosomal protein S6



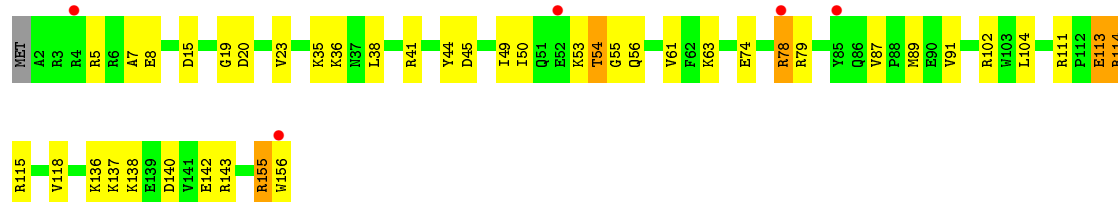
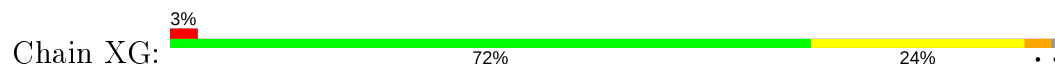
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

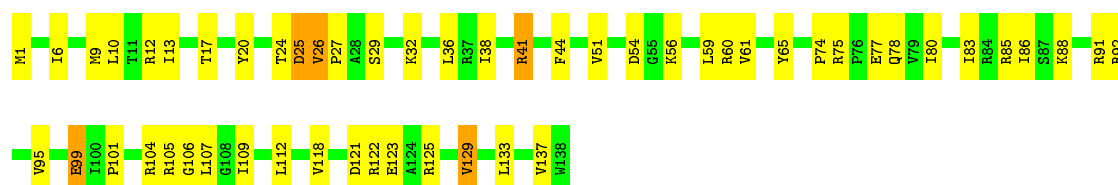


• Molecule 7: 30S ribosomal protein S7



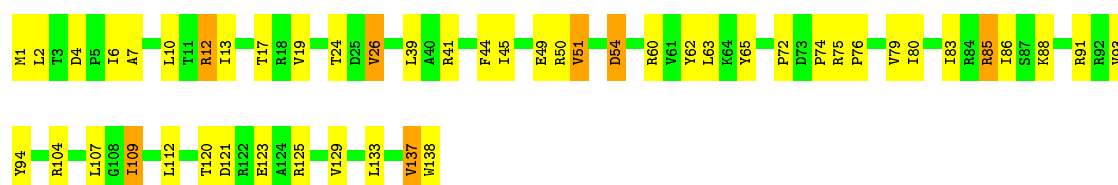
- Molecule 8: 30S ribosomal protein S8

Chain QH: 



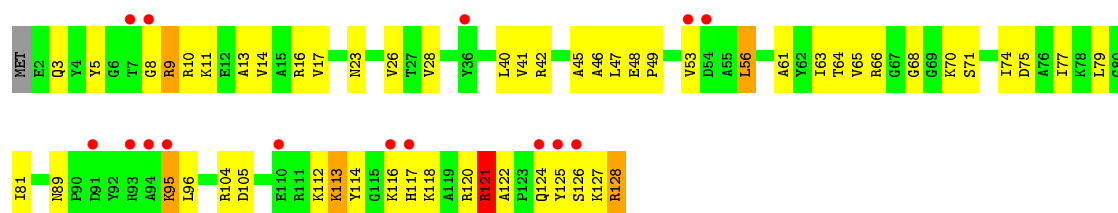
- Molecule 8: 30S ribosomal protein S8

Chain XH: 



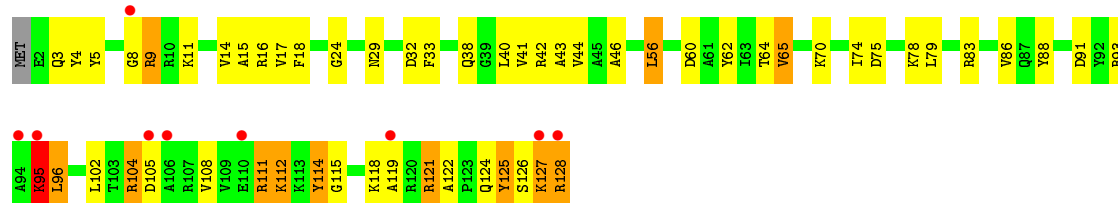
- Molecule 9: 30S ribosomal protein S9

Chain QI: 



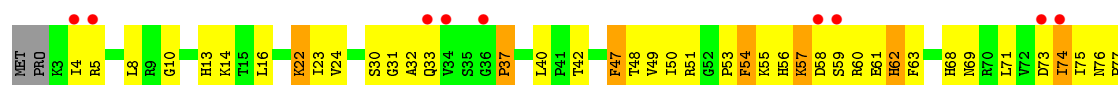
- Molecule 9: 30S ribosomal protein S9

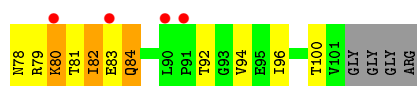
Chain XI: 



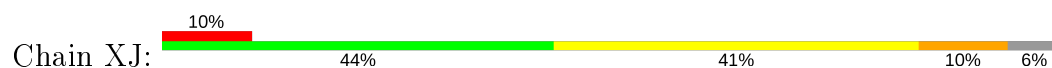
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 

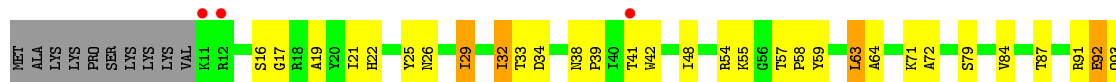




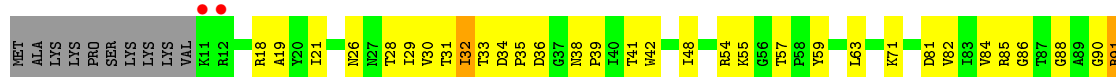
- Molecule 10: 30S ribosomal protein S10



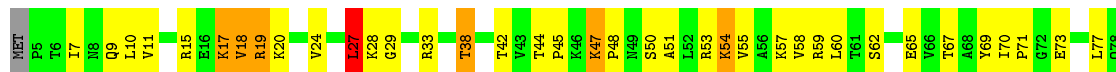
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

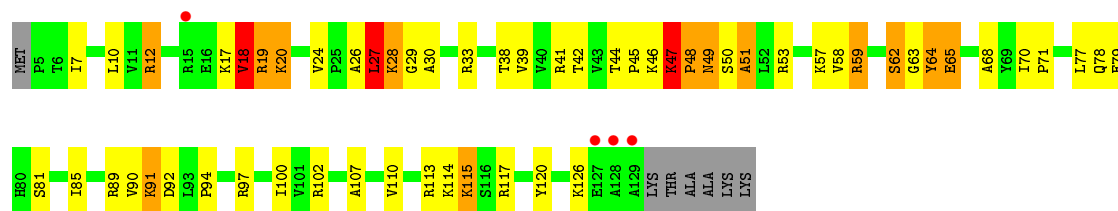


- Molecule 12: 30S ribosomal protein S12

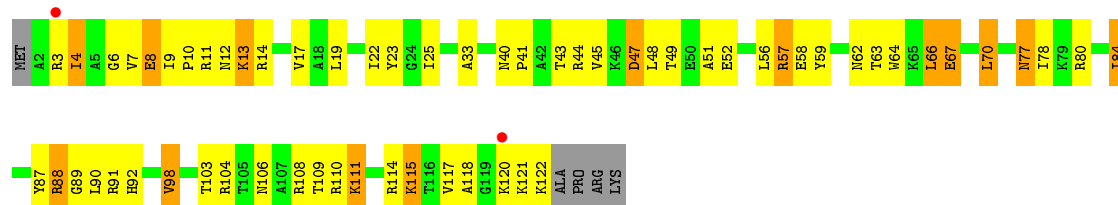


- Molecule 12: 30S ribosomal protein S12

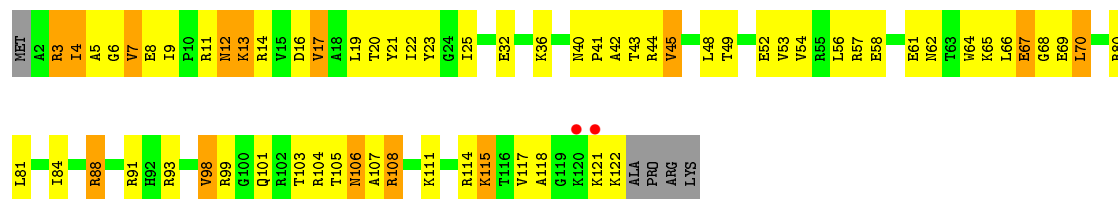




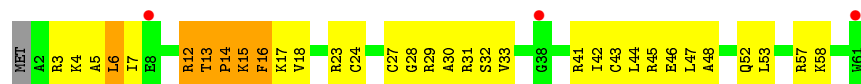
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



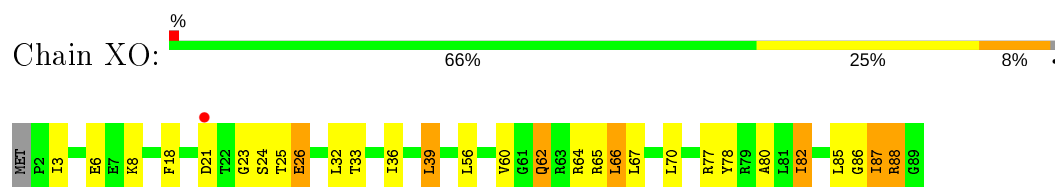
- Molecule 14: 30S ribosomal protein S14 type Z



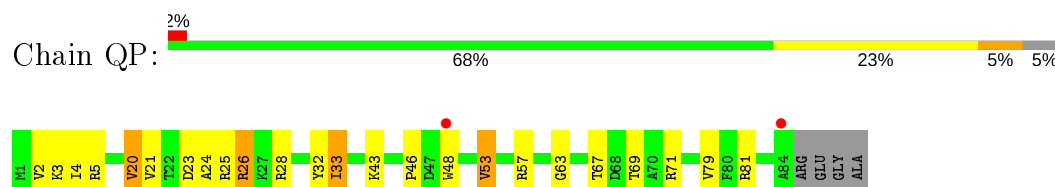
- Molecule 15: 30S ribosomal protein S15



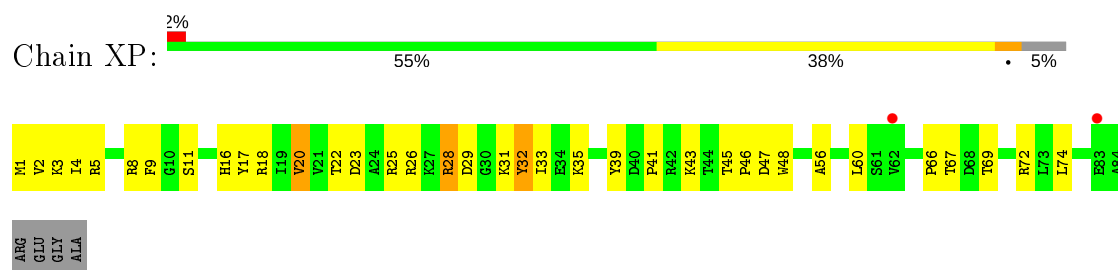
- Molecule 15: 30S ribosomal protein S15



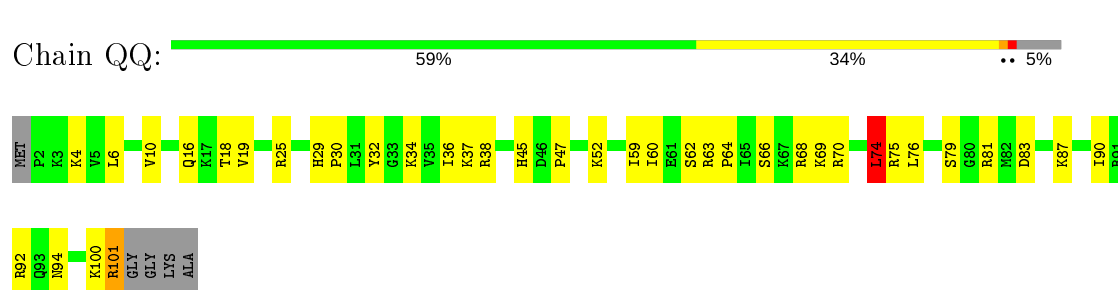
- Molecule 16: 30S ribosomal protein S16



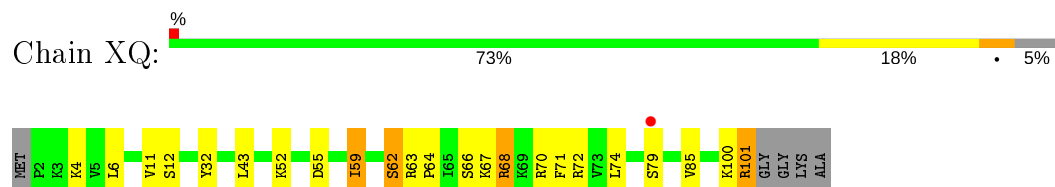
- Molecule 16: 30S ribosomal protein S16



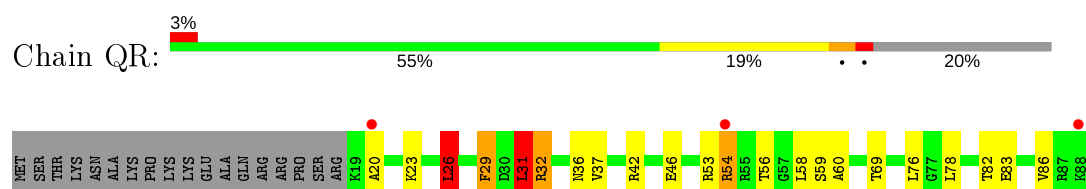
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

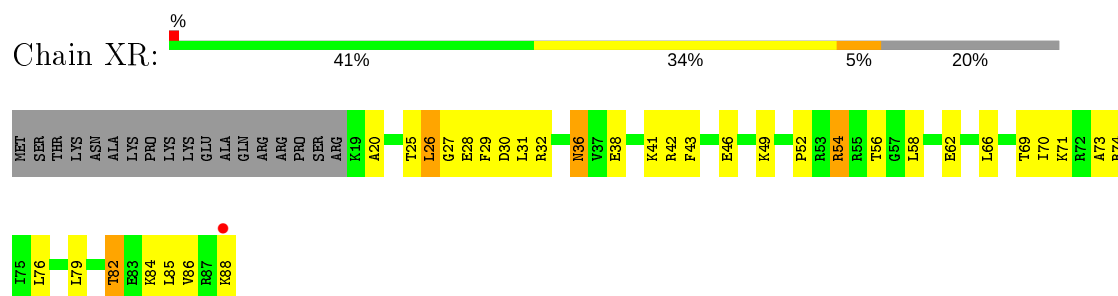


- Molecule 18: 30S ribosomal protein S18

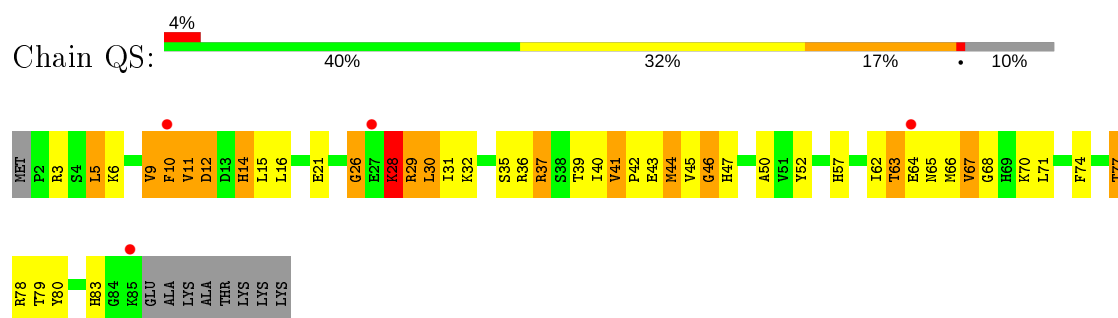




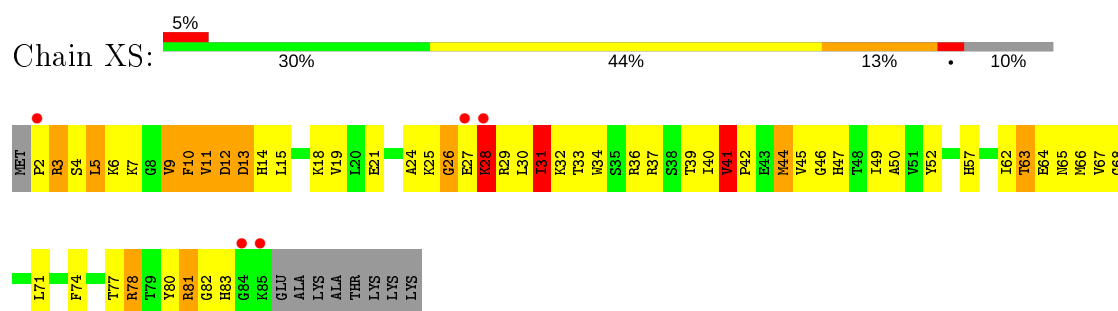
- Molecule 18: 30S ribosomal protein S18



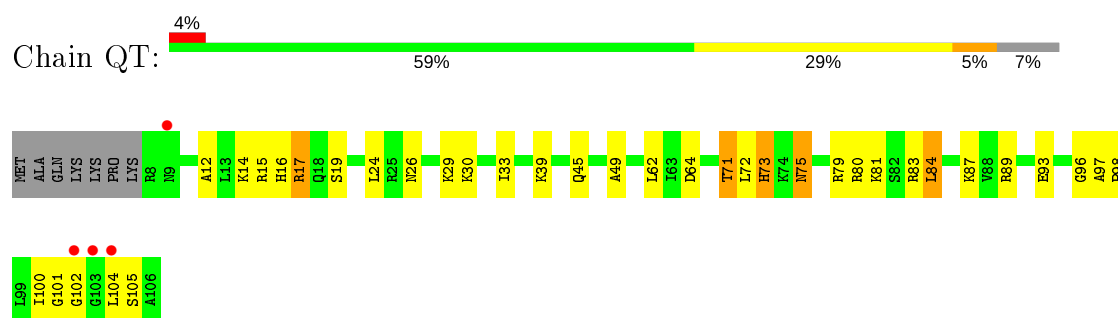
- Molecule 19: 30S ribosomal protein S19



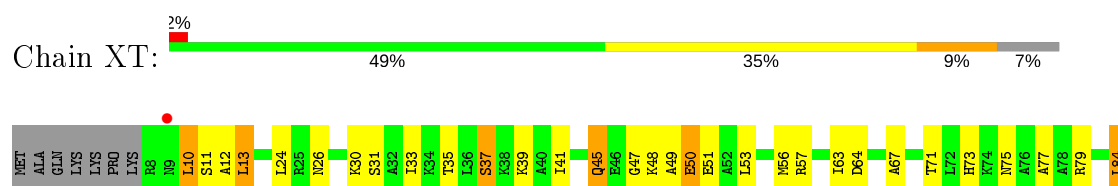
- Molecule 19: 30S ribosomal protein S19

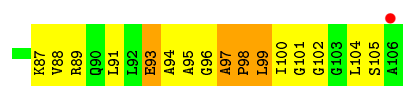


- Molecule 20: 30S ribosomal protein S20

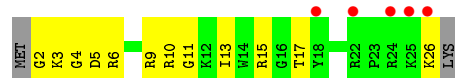


- Molecule 20: 30S ribosomal protein S20

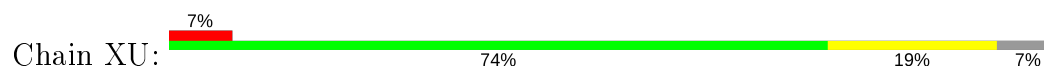




- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



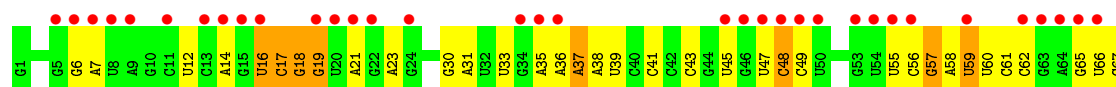
- Molecule 22: tRNA-fMet



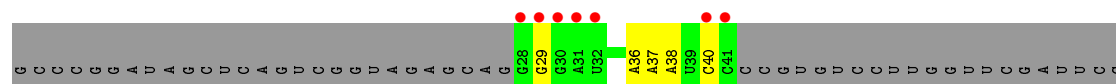
- Molecule 22: tRNA-fMet



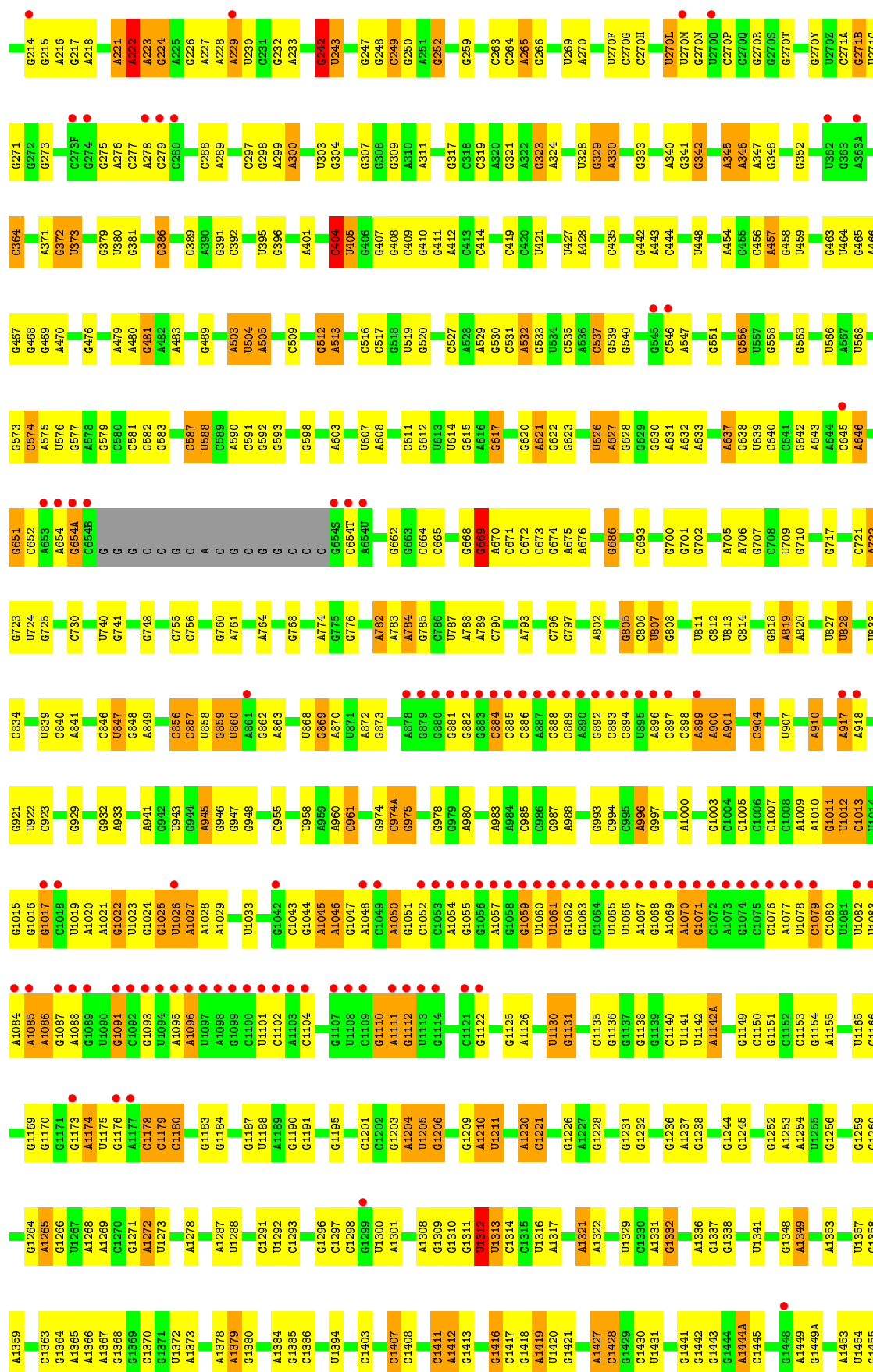
- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe



- Molecule 23: E-Site tRNA-Phe or A-Site tRNA-Phe

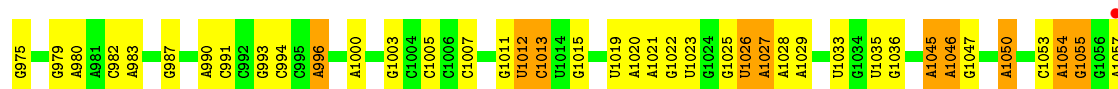




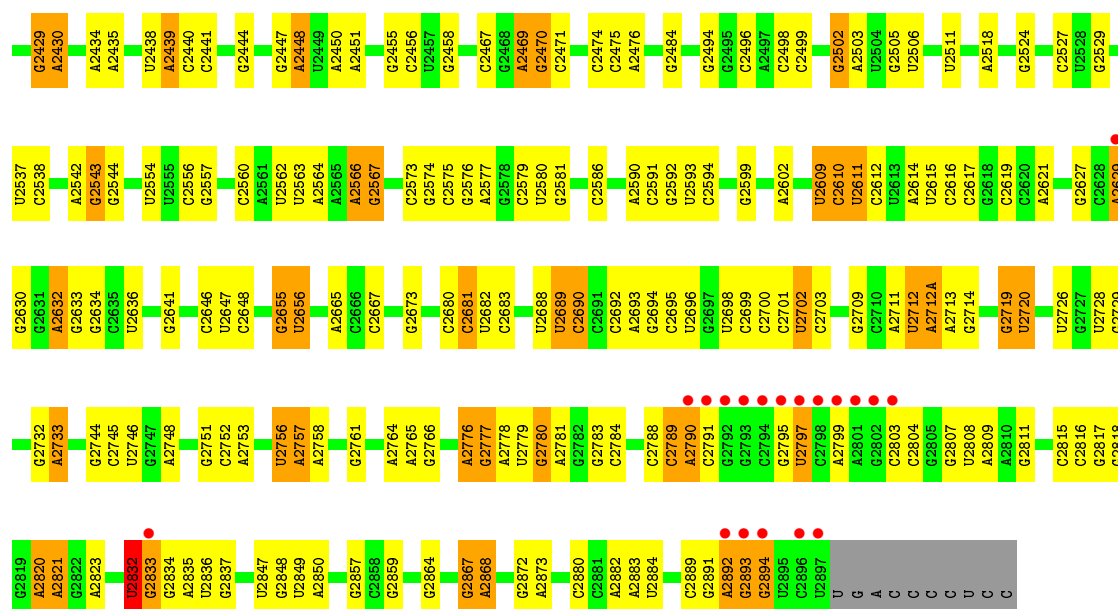




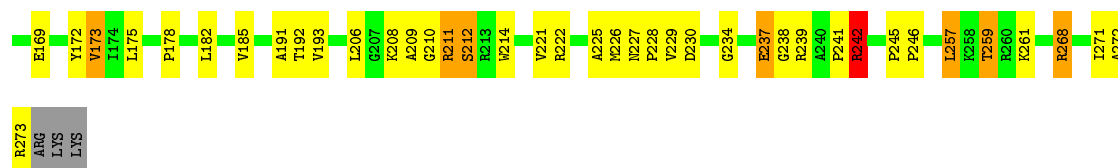
- Molecule 25: 23S ribosomal RNA



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

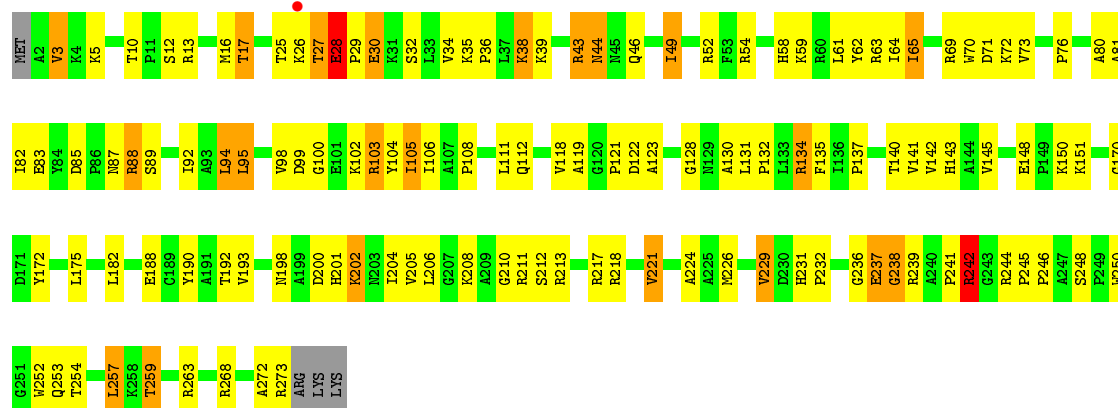






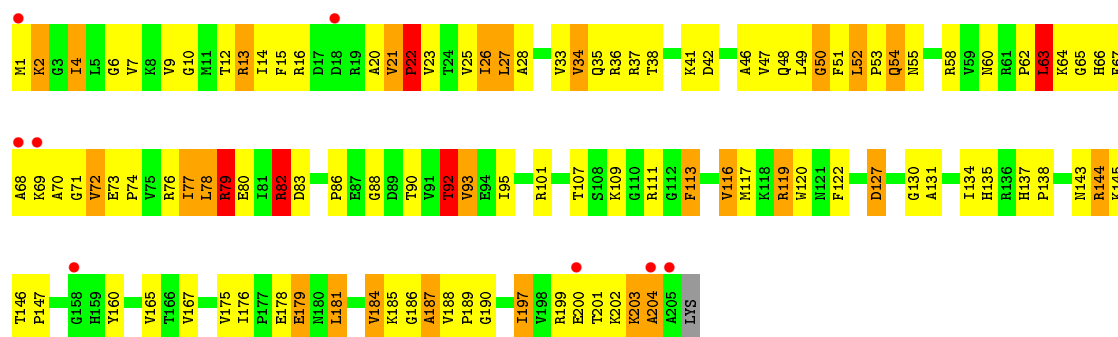
• Molecule 27: 50S ribosomal protein L2

Chain YD: 52% 38% 8% ..



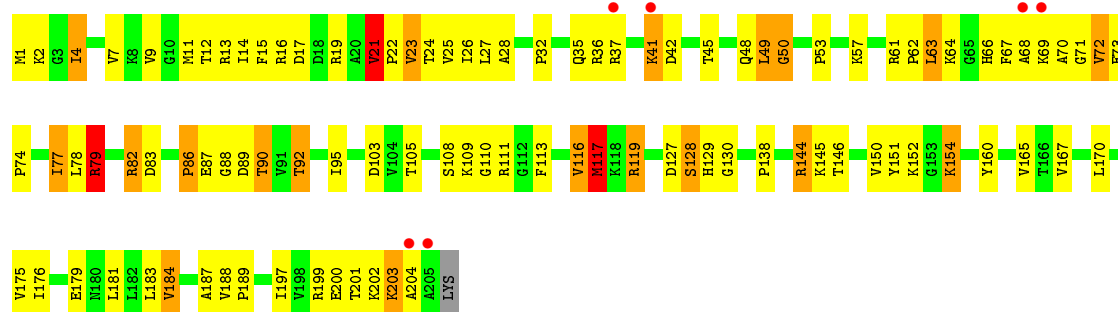
• Molecule 28: 50S ribosomal protein L3

Chain RE: 4% 46% 38% 13% .

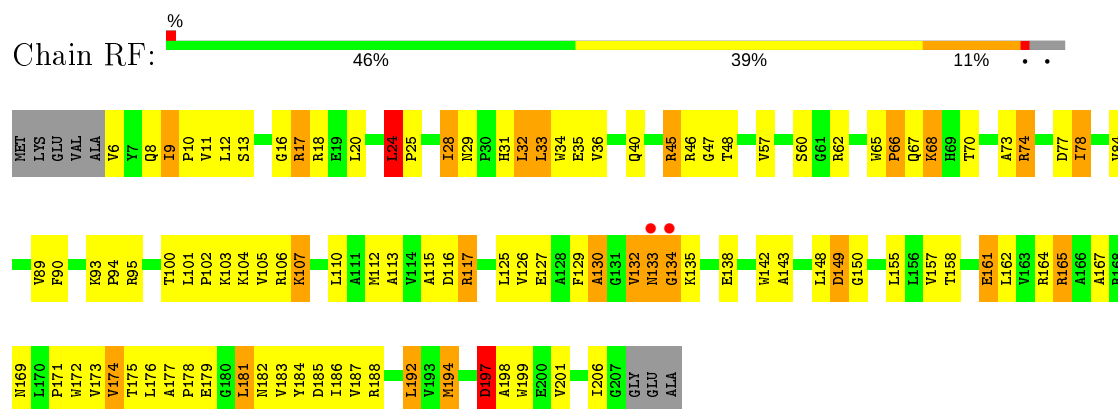


• Molecule 28: 50S ribosomal protein L3

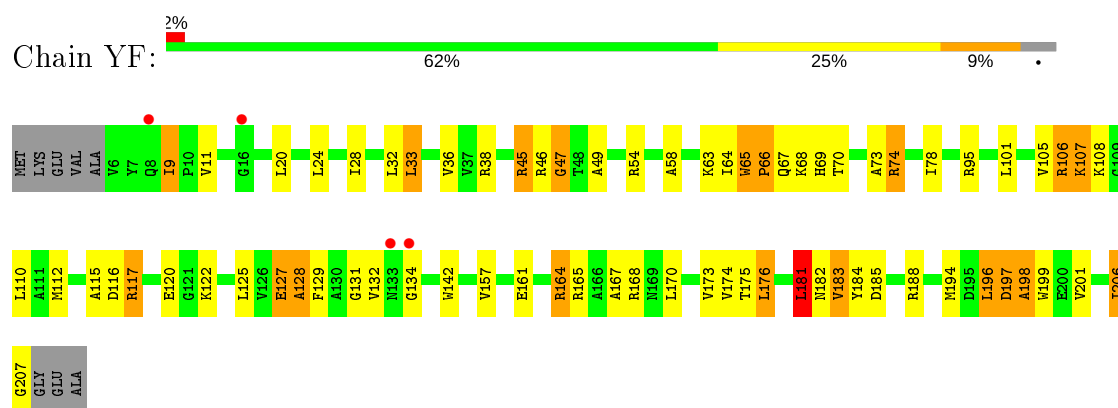
Chain YE: 3% 51% 38% 9% .



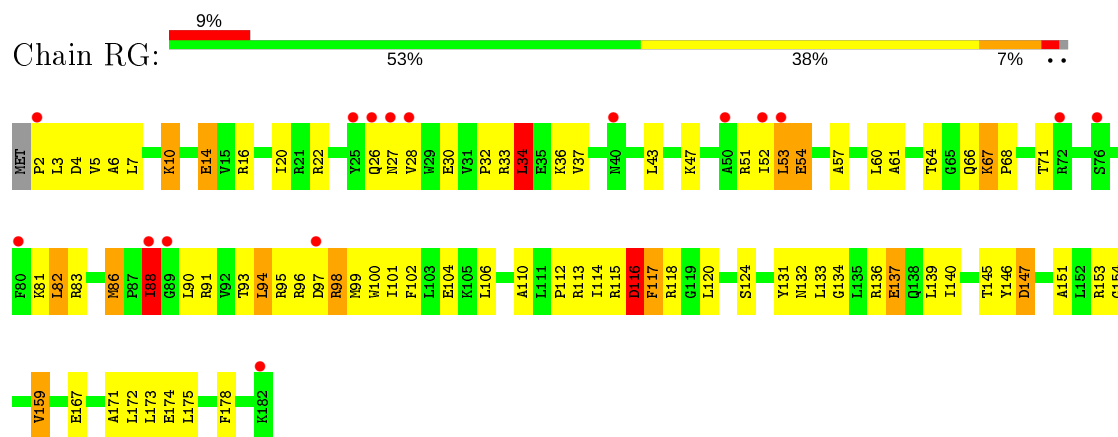
- Molecule 29: 50S ribosomal protein L4



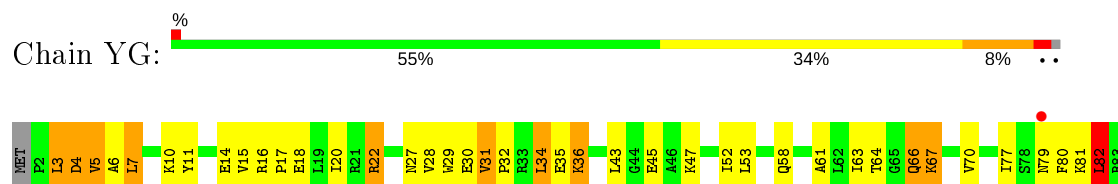
- Molecule 29: 50S ribosomal protein L4

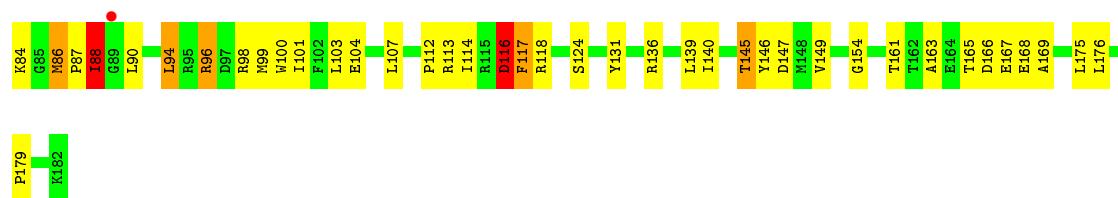


- Molecule 30: 50S ribosomal protein L5

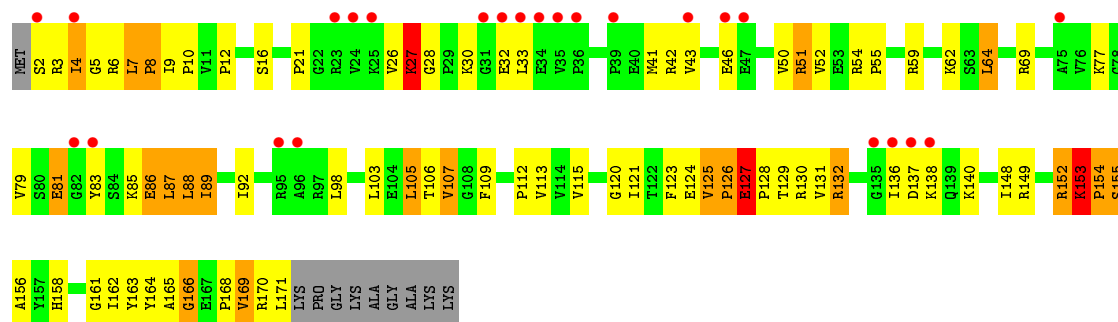


- Molecule 30: 50S ribosomal protein L5

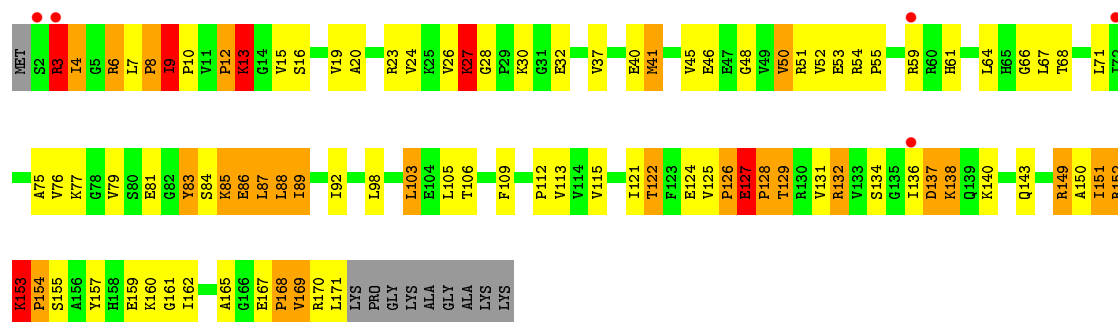
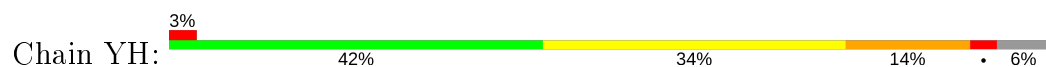




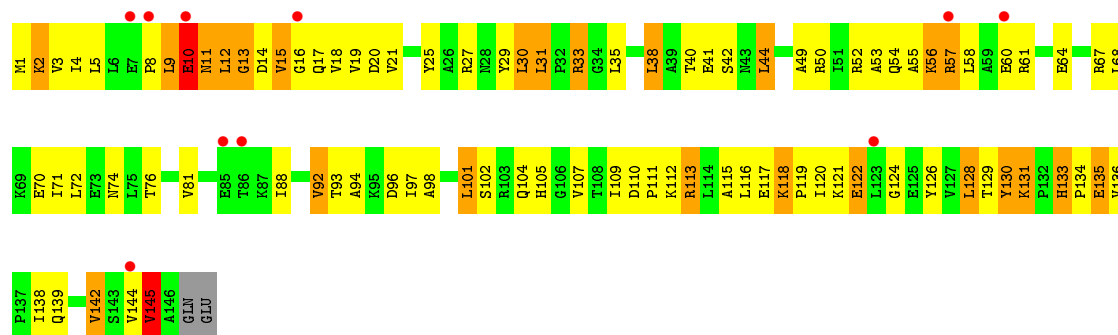
- Molecule 31: 50S ribosomal protein L6



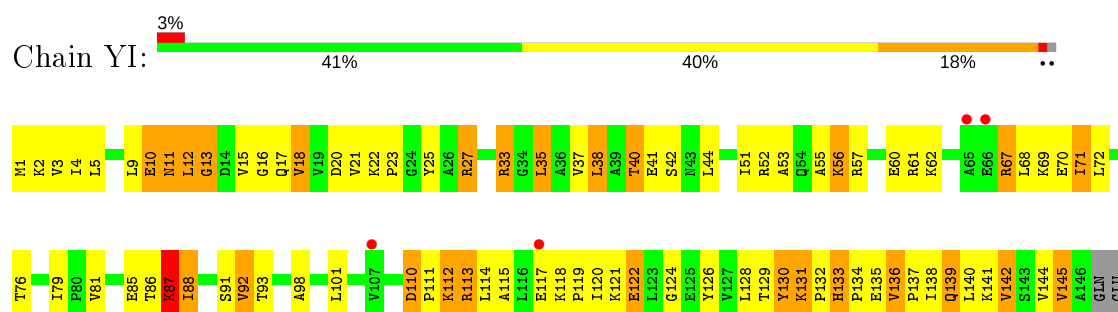
- Molecule 31: 50S ribosomal protein L6



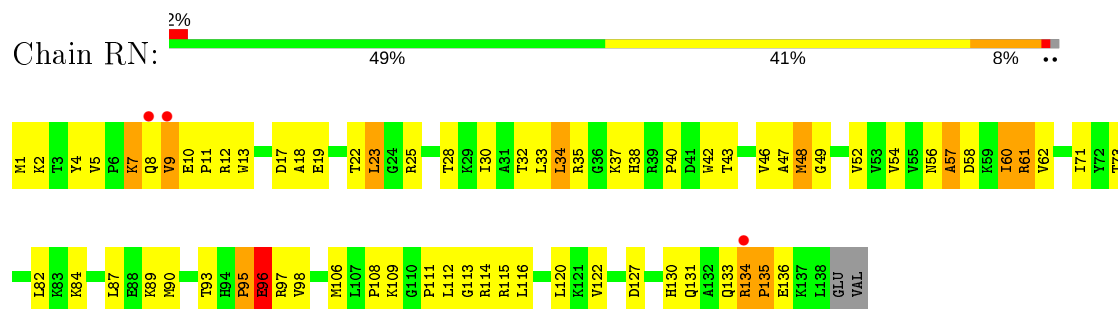
- Molecule 32: 50S ribosomal protein L9



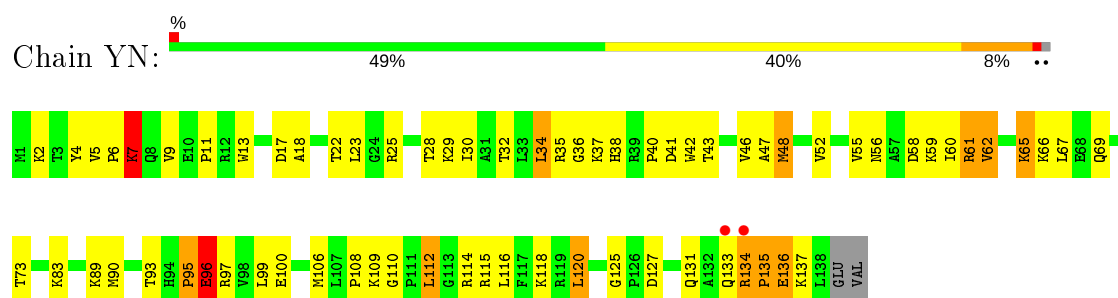
- Molecule 32: 50S ribosomal protein L9



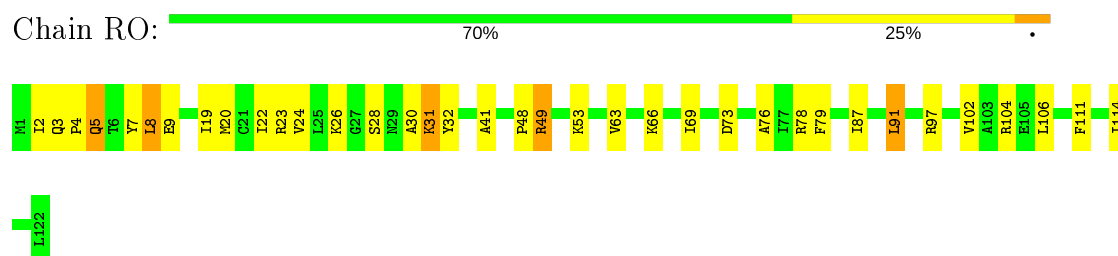
- Molecule 33: 50S ribosomal protein L13

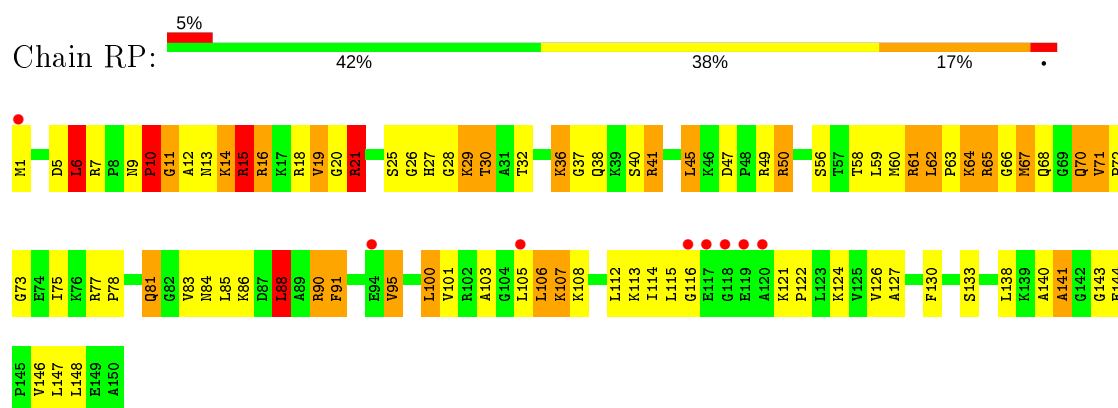


- Molecule 33: 50S ribosomal protein L13

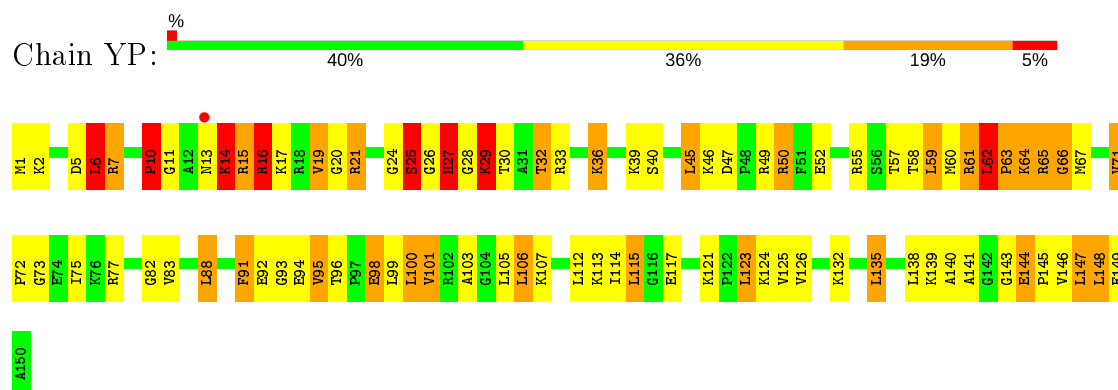


- Molecule 34: 50S ribosomal protein L14

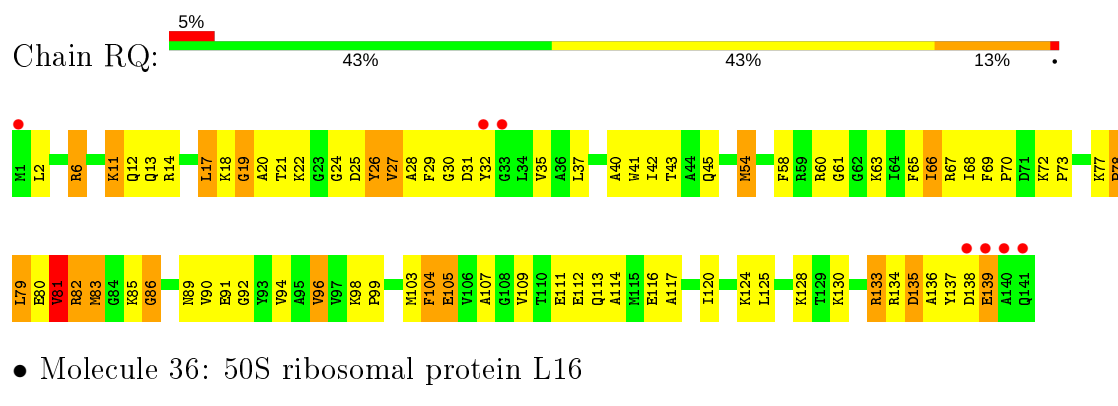




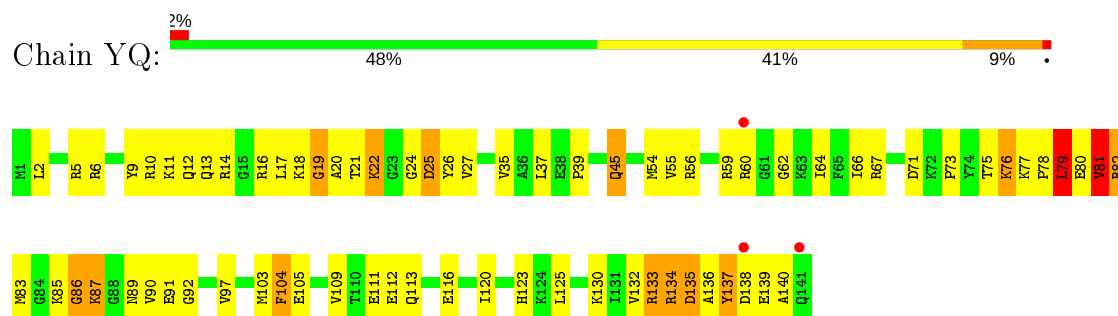
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

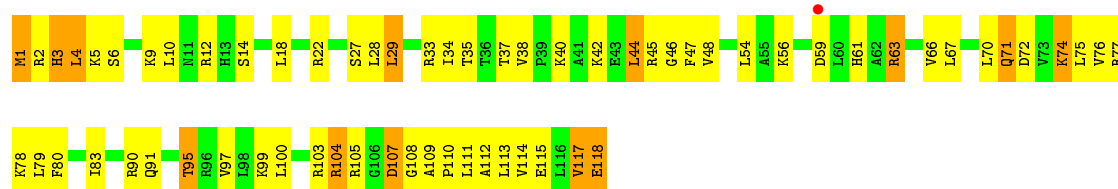


• Molecule 36: 50S ribosomal protein L16

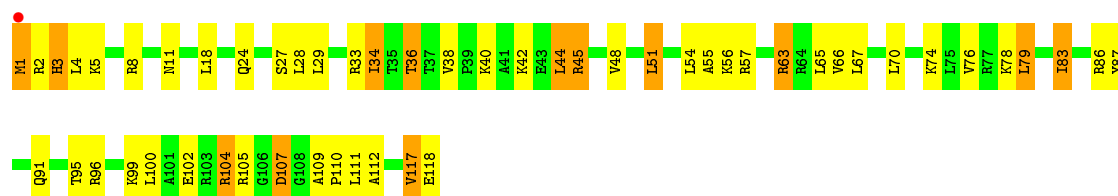


• Molecule 37: 50S ribosomal protein L17

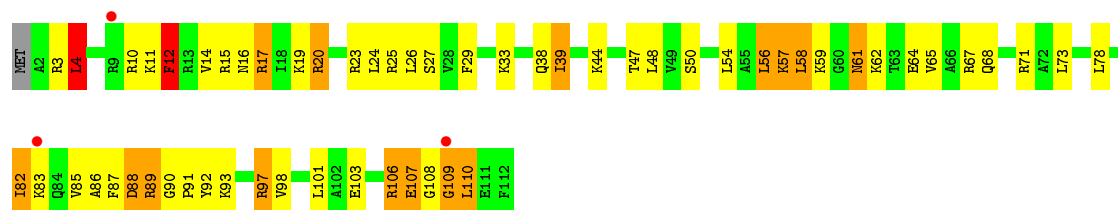




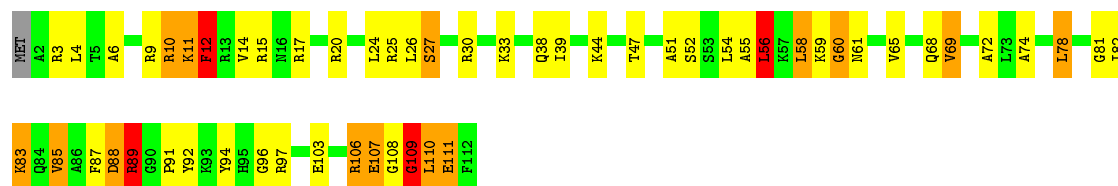
• Molecule 37: 50S ribosomal protein L17



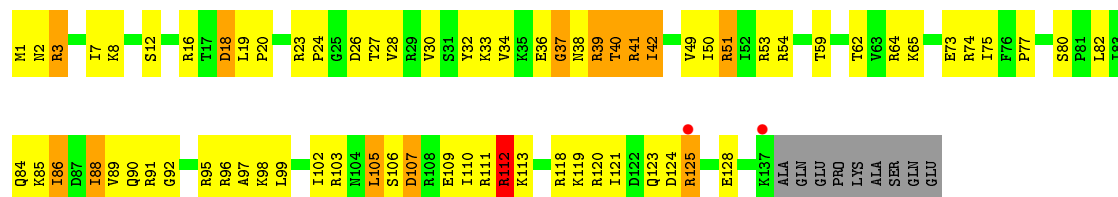
• Molecule 38: 50S ribosomal protein L18



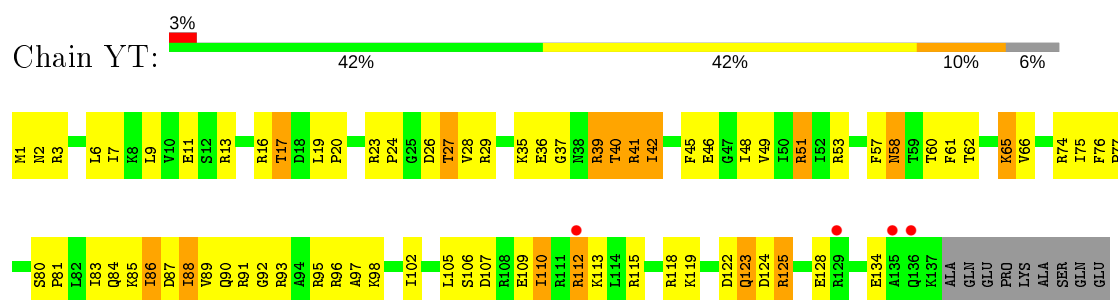
• Molecule 38: 50S ribosomal protein L18



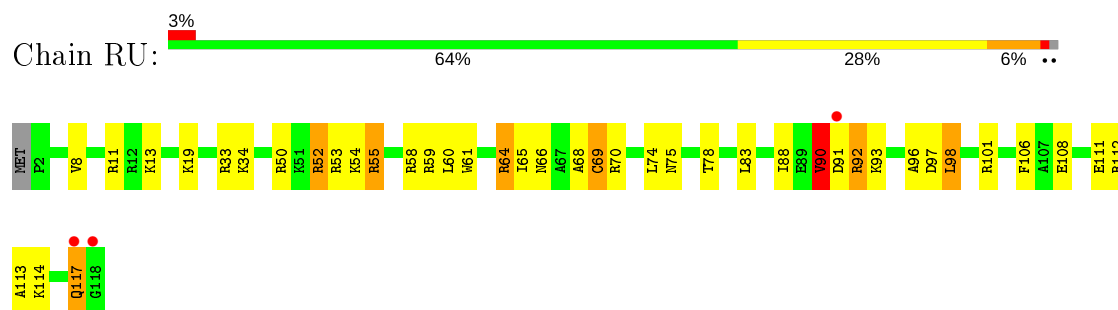
• Molecule 39: 50S ribosomal protein L19



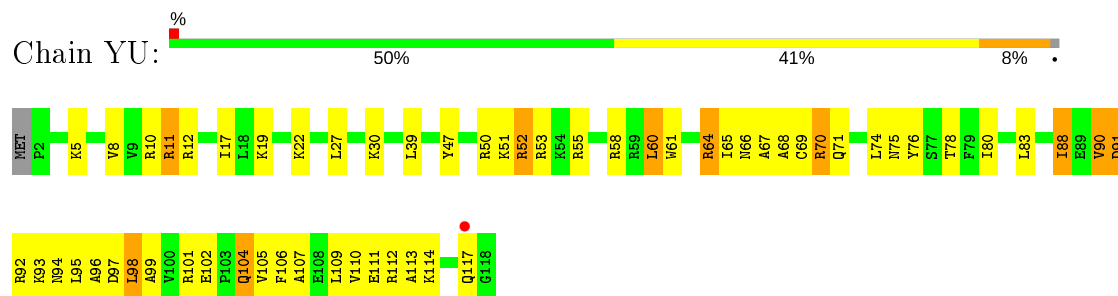
• Molecule 39: 50S ribosomal protein L19



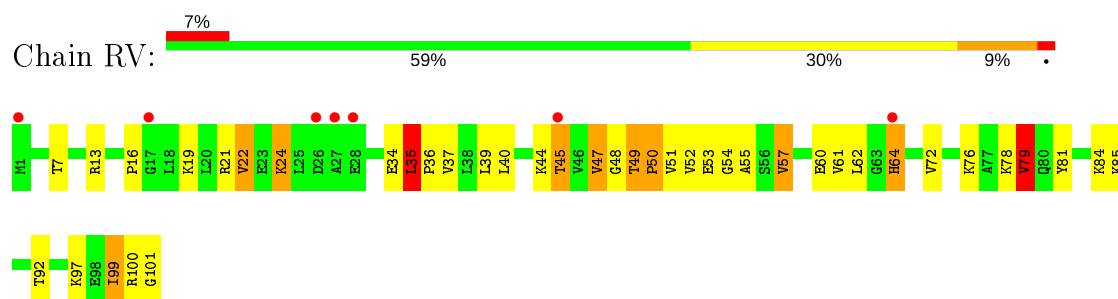
- Molecule 40: 50S ribosomal protein L20



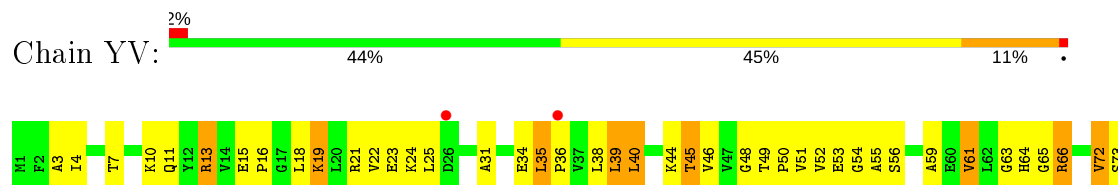
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21





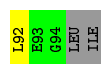
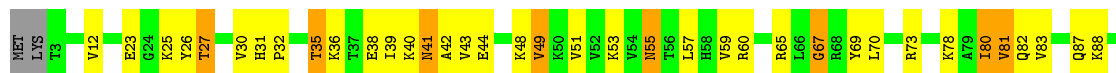
- Molecule 42: 50S ribosomal protein L22



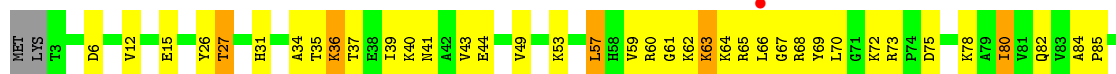
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23



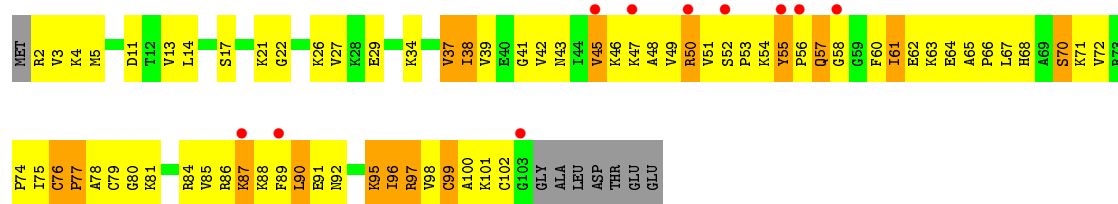
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24



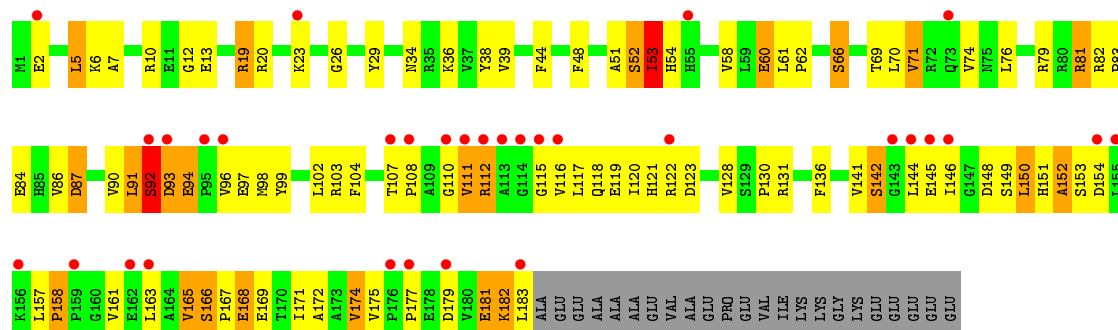
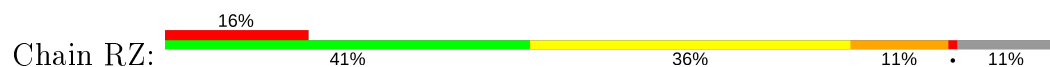




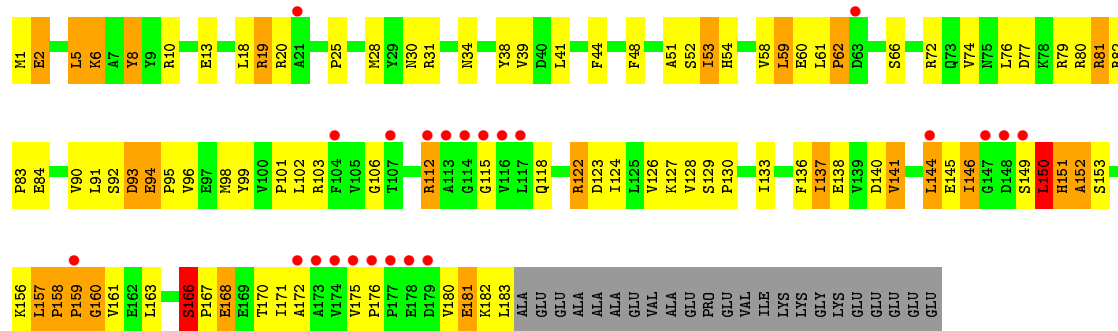
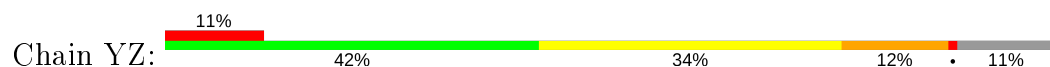
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27

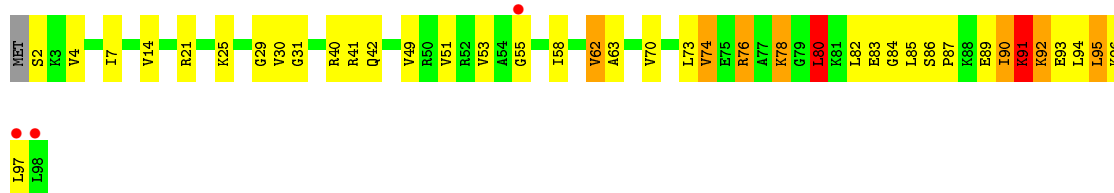




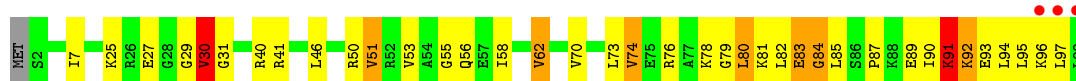
- Molecule 46: 50S ribosomal protein L27



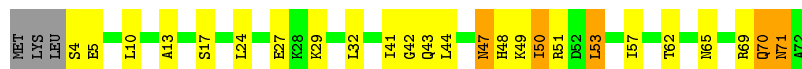
- Molecule 47: 50S ribosomal protein L28



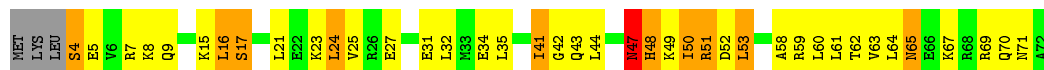
- Molecule 47: 50S ribosomal protein L28



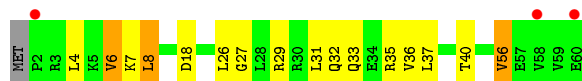
- Molecule 48: 50S ribosomal protein L29



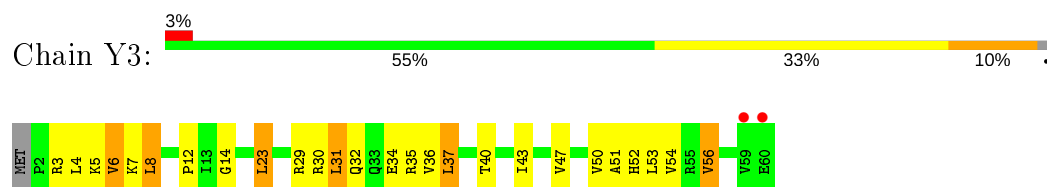
- Molecule 48: 50S ribosomal protein L29



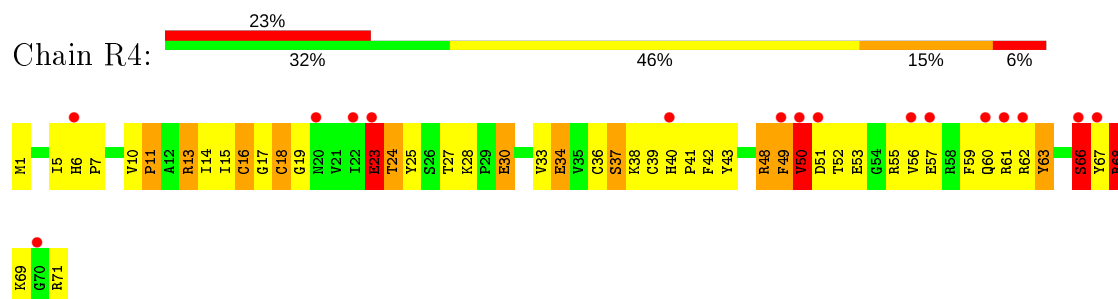
- Molecule 49: 50S ribosomal protein L30



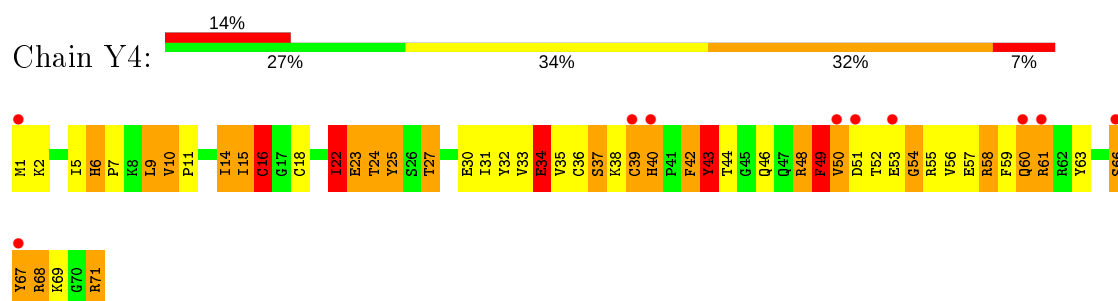
- Molecule 49: 50S ribosomal protein L30



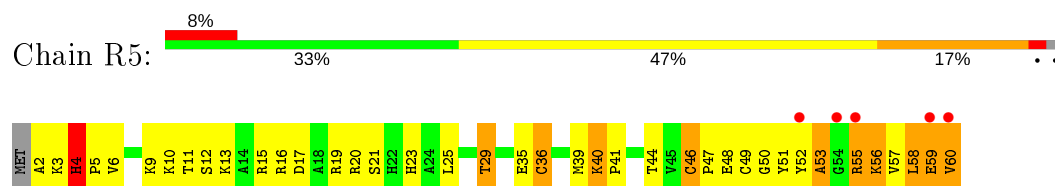
- Molecule 50: 50S ribosomal protein L31



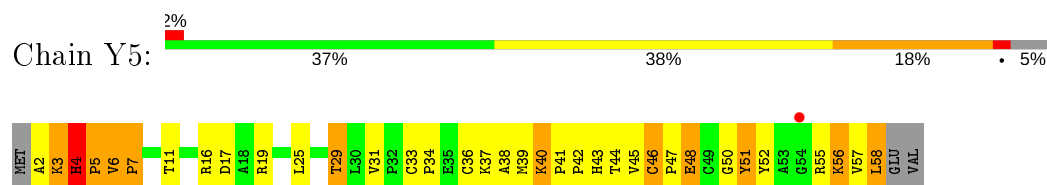
- Molecule 50: 50S ribosomal protein L31



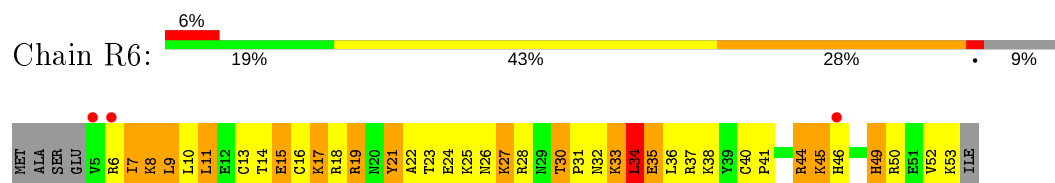
- Molecule 51: 50S ribosomal protein L32



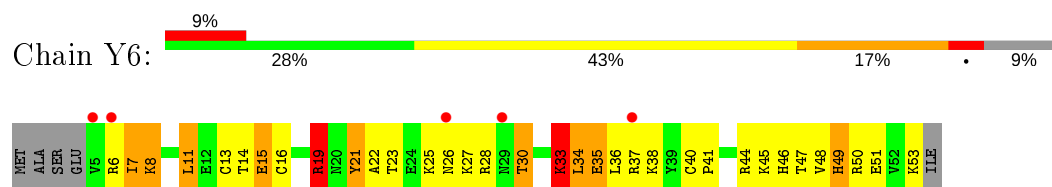
- Molecule 51: 50S ribosomal protein L32



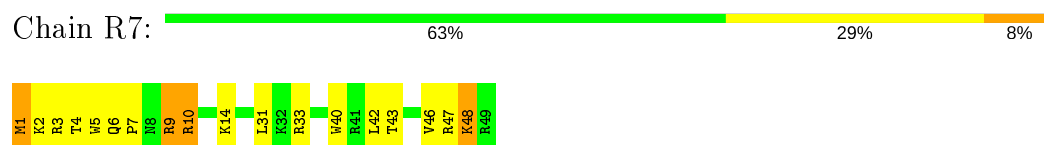
- Molecule 52: 50S ribosomal protein L33



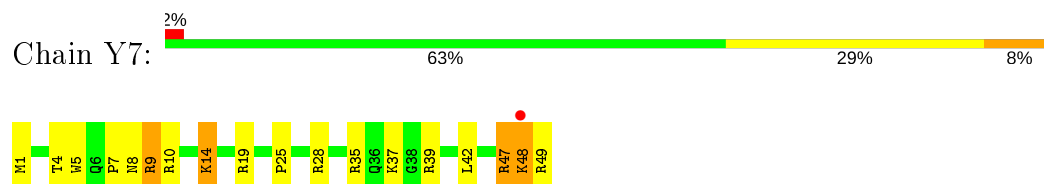
- Molecule 52: 50S ribosomal protein L33



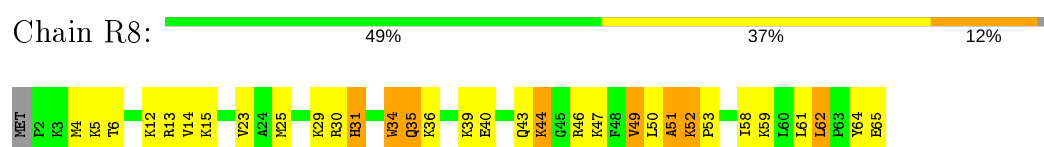
- Molecule 53: 50S ribosomal protein L34



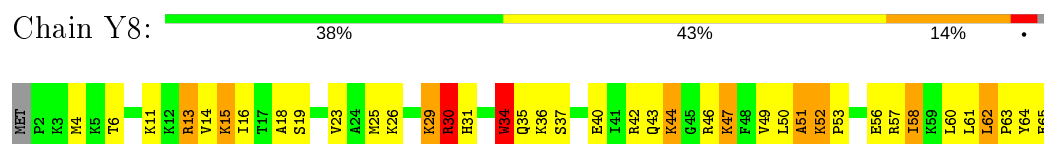
- Molecule 53: 50S ribosomal protein L34



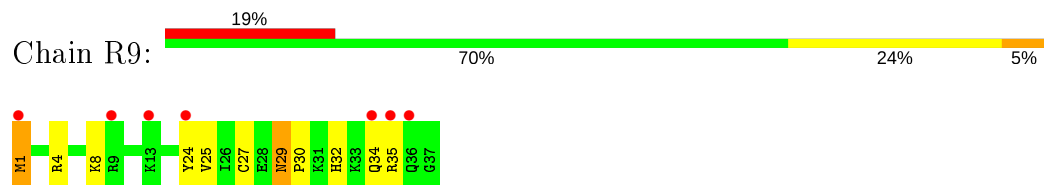
- Molecule 54: 50S ribosomal protein L35



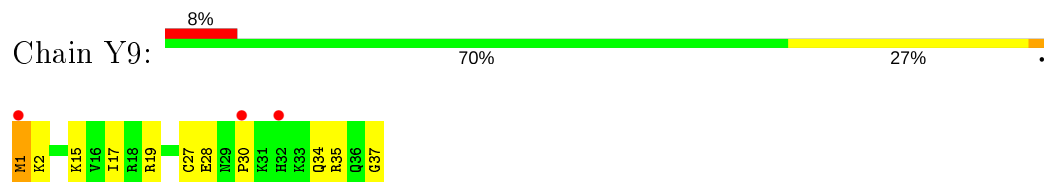
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



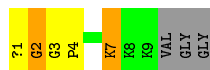
- Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain Z7:  17% 58% 25%



- Molecule 56: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain Z8:  33% 25% 17% 25%



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.24Å 443.46Å 618.62Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.79 – 3.60<br>34.94 – 3.61                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.1 (49.79-3.60)<br>98.0 (34.94-3.61)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.74 (at 3.66Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.3_1479)                          | Depositor        |
| R, $R_{free}$   | 0.222 , 0.254<br>0.224 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set   | 28952 reflections (4.54%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 104.1   | Xtriage          |
| Anisotropy  | 0.244   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 79.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 295487  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 109.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: ZN, MG, T17, PAR

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

| Mol | Chain | Bond lengths |              | Bond angles |                 |
|-----|-------|--------------|--------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$  | RMSZ        | # $ Z  > 5$     |
| 1   | QA    | 0.23         | 0/36098      | 0.81        | 32/56341 (0.1%) |
| 1   | XA    | 0.24         | 0/36101      | 0.81        | 18/56346 (0.0%) |
| 2   | QB    | 0.31         | 0/1959       | 0.52        | 0/2642          |
| 2   | XB    | 0.32         | 0/1959       | 0.54        | 0/2642          |
| 3   | QC    | 0.32         | 0/1629       | 0.53        | 0/2195          |
| 3   | XC    | 0.37         | 0/1629       | 0.56        | 0/2195          |
| 4   | QD    | 0.45         | 0/1733       | 0.62        | 1/2318 (0.0%)   |
| 4   | XD    | 0.39         | 0/1733       | 0.60        | 0/2318          |
| 5   | QE    | 0.35         | 0/1171       | 0.56        | 0/1576          |
| 5   | XE    | 0.39         | 0/1171       | 0.59        | 0/1576          |
| 6   | QF    | 0.39         | 0/856        | 0.57        | 0/1154          |
| 6   | XF    | 0.39         | 0/856        | 0.61        | 0/1154          |
| 7   | QG    | 0.33         | 0/1276       | 0.50        | 0/1709          |
| 7   | XG    | 0.34         | 0/1276       | 0.51        | 0/1709          |
| 8   | QH    | 0.33         | 0/1136       | 0.55        | 0/1527          |
| 8   | XH    | 0.38         | 0/1136       | 0.58        | 0/1527          |
| 9   | QI    | 0.31         | 0/1029       | 0.55        | 0/1379          |
| 9   | XI    | 0.34         | 0/1029       | 0.58        | 0/1379          |
| 10  | QJ    | 0.33         | 0/814        | 0.54        | 0/1095          |
| 10  | XJ    | 0.35         | 0/814        | 0.60        | 0/1095          |
| 11  | QK    | 0.37         | 0/900        | 0.57        | 0/1213          |
| 11  | XK    | 0.39         | 0/900        | 0.58        | 0/1213          |
| 12  | QL    | 0.37         | 0/991        | 0.61        | 0/1327          |
| 12  | XL    | 0.50         | 1/991 (0.1%) | 0.77        | 2/1327 (0.2%)   |
| 13  | QM    | 0.32         | 0/974        | 0.59        | 0/1303          |
| 13  | XM    | 0.36         | 0/974        | 0.63        | 0/1303          |
| 14  | QN    | 0.40         | 0/501        | 0.60        | 0/664           |
| 14  | XN    | 0.42         | 0/501        | 0.66        | 0/664           |
| 15  | QO    | 0.35         | 0/745        | 0.53        | 0/992           |
| 15  | XO    | 0.39         | 0/745        | 0.54        | 0/992           |
| 16  | QP    | 0.36         | 0/721        | 0.57        | 0/970           |
| 16  | XP    | 0.35         | 0/721        | 0.57        | 0/970           |

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5          |
| 17  | QQ    | 0.35         | 0/847         | 0.53        | 0/1131           |
| 17  | XQ    | 0.35         | 0/847         | 0.54        | 0/1131           |
| 18  | QR    | 0.35         | 0/579         | 0.64        | 1/768 (0.1%)     |
| 18  | XR    | 0.37         | 0/579         | 0.60        | 0/768            |
| 19  | QS    | 0.33         | 0/689         | 0.60        | 0/926            |
| 19  | XS    | 0.38         | 0/689         | 0.69        | 1/926 (0.1%)     |
| 20  | QT    | 0.36         | 0/765         | 0.64        | 0/1007           |
| 20  | XT    | 0.31         | 0/765         | 0.60        | 0/1007           |
| 21  | QU    | 0.31         | 0/221         | 0.53        | 0/288            |
| 21  | XU    | 0.32         | 0/221         | 0.61        | 0/288            |
| 22  | QV    | 0.32         | 1/1836 (0.1%) | 0.80        | 0/2859           |
| 22  | XV    | 0.33         | 1/1836 (0.1%) | 0.81        | 1/2859 (0.0%)    |
| 23  | QW    | 0.19         | 0/1809        | 0.79        | 0/2819           |
| 23  | QY    | 0.17         | 0/406         | 0.73        | 0/628            |
| 23  | XW    | 0.20         | 0/1809        | 0.80        | 0/2819           |
| 23  | XY    | 0.20         | 0/406         | 0.74        | 0/628            |
| 24  | QX    | 0.19         | 0/235         | 0.71        | 0/364            |
| 24  | XX    | 0.18         | 0/235         | 0.65        | 0/364            |
| 25  | RA    | 0.26         | 0/69521       | 0.81        | 28/108529 (0.0%) |
| 25  | YA    | 0.29         | 0/69543       | 0.83        | 41/108563 (0.0%) |
| 26  | RB    | 0.26         | 0/2878        | 0.88        | 7/4490 (0.2%)    |
| 26  | YB    | 0.29         | 0/2878        | 0.91        | 11/4490 (0.2%)   |
| 27  | RD    | 0.51         | 0/2165        | 0.70        | 0/2919           |
| 27  | YD    | 0.57         | 0/2165        | 0.77        | 1/2919 (0.0%)    |
| 28  | RE    | 0.46         | 1/1601 (0.1%) | 0.73        | 3/2160 (0.1%)    |
| 28  | YE    | 0.48         | 1/1601 (0.1%) | 0.74        | 2/2160 (0.1%)    |
| 29  | RF    | 0.45         | 1/1620 (0.1%) | 0.64        | 1/2194 (0.0%)    |
| 29  | YF    | 0.48         | 0/1620        | 0.71        | 1/2194 (0.0%)    |
| 30  | RG    | 0.31         | 0/1499        | 0.57        | 1/2016 (0.0%)    |
| 30  | YG    | 0.40         | 0/1499        | 0.60        | 0/2016           |
| 31  | RH    | 0.33         | 1/1332 (0.1%) | 0.73        | 2/1802 (0.1%)    |
| 31  | YH    | 0.50         | 1/1332 (0.1%) | 0.76        | 2/1802 (0.1%)    |
| 32  | RI    | 0.40         | 0/1151        | 0.75        | 1/1558 (0.1%)    |
| 32  | YI    | 0.38         | 0/1151        | 0.66        | 0/1558           |
| 33  | RN    | 0.41         | 0/1131        | 0.62        | 0/1525           |
| 33  | YN    | 0.43         | 0/1131        | 0.64        | 0/1525           |
| 34  | RO    | 0.41         | 0/943         | 0.62        | 1/1269 (0.1%)    |
| 34  | YO    | 0.50         | 0/943         | 0.65        | 0/1269           |
| 35  | RP    | 0.48         | 1/1162 (0.1%) | 0.83        | 1/1544 (0.1%)    |
| 35  | YP    | 0.55         | 2/1162 (0.2%) | 0.93        | 4/1544 (0.3%)    |
| 36  | RQ    | 0.44         | 0/1143        | 0.71        | 1/1527 (0.1%)    |
| 36  | YQ    | 0.56         | 0/1143        | 0.78        | 0/1527           |
| 37  | RR    | 0.42         | 0/982         | 0.69        | 0/1312           |



| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 37  | YR    | 0.45         | 0/982            | 0.73        | 0/1312            |
| 38  | RS    | 0.36         | 0/892            | 0.64        | 0/1187            |
| 38  | YS    | 0.39         | 0/892            | 0.71        | 0/1187            |
| 39  | RT    | 0.41         | 0/1155           | 0.63        | 0/1542            |
| 39  | YT    | 0.44         | 0/1155           | 0.67        | 0/1542            |
| 40  | RU    | 0.40         | 0/982            | 0.65        | 0/1306            |
| 40  | YU    | 0.50         | 0/982            | 0.69        | 0/1306            |
| 41  | RV    | 0.38         | 0/790            | 0.61        | 1/1057 (0.1%)     |
| 41  | YV    | 0.46         | 0/790            | 0.73        | 1/1057 (0.1%)     |
| 42  | RW    | 0.50         | 0/911            | 0.67        | 0/1220            |
| 42  | YW    | 0.45         | 0/911            | 0.68        | 0/1220            |
| 43  | RX    | 0.47         | 0/739            | 0.62        | 0/993             |
| 43  | YX    | 0.50         | 0/739            | 0.66        | 0/993             |
| 44  | RY    | 0.44         | 0/798            | 0.68        | 0/1064            |
| 44  | YY    | 0.45         | 0/798            | 0.69        | 0/1064            |
| 45  | RZ    | 0.34         | 0/1493           | 0.60        | 0/2026            |
| 45  | YZ    | 0.45         | 2/1493 (0.1%)    | 0.68        | 4/2026 (0.2%)     |
| 46  | R0    | 0.45         | 0/657            | 0.65        | 0/874             |
| 46  | Y0    | 0.48         | 0/657            | 0.69        | 0/874             |
| 47  | R1    | 0.44         | 0/770            | 0.66        | 0/1022            |
| 47  | Y1    | 0.46         | 0/770            | 0.69        | 0/1022            |
| 48  | R2    | 0.39         | 0/583            | 0.65        | 0/771             |
| 48  | Y2    | 0.52         | 0/583            | 0.73        | 0/771             |
| 49  | R3    | 0.35         | 0/474            | 0.57        | 0/635             |
| 49  | Y3    | 0.41         | 0/474            | 0.59        | 0/635             |
| 50  | R4    | 0.33         | 0/594            | 0.68        | 0/795             |
| 50  | Y4    | 0.37         | 0/594            | 0.69        | 0/795             |
| 51  | R5    | 0.43         | 0/473            | 0.78        | 0/639             |
| 51  | Y5    | 0.68         | 3/456 (0.7%)     | 0.89        | 3/617 (0.5%)      |
| 52  | R6    | 0.35         | 0/431            | 0.69        | 0/575             |
| 52  | Y6    | 0.37         | 0/431            | 0.68        | 0/575             |
| 53  | R7    | 0.49         | 0/438            | 0.68        | 0/575             |
| 53  | Y7    | 0.57         | 0/438            | 0.71        | 0/575             |
| 54  | R8    | 0.55         | 0/525            | 0.79        | 0/691             |
| 54  | Y8    | 0.58         | 0/525            | 0.82        | 0/691             |
| 55  | R9    | 0.26         | 0/310            | 0.45        | 0/407             |
| 55  | Y9    | 0.32         | 0/310            | 0.48        | 0/407             |
| 56  | Z7    | 0.22         | 0/56             | 0.45        | 0/70              |
| 56  | Z8    | 0.25         | 0/56             | 0.45        | 0/70              |
| All | All   | 0.32         | 16/320246 (0.0%) | 0.78        | 173/478995 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 12  | QL    | 0                   | 1                   |
| 12  | XL    | 0                   | 1                   |
| 29  | YF    | 0                   | 1                   |
| 31  | RH    | 0                   | 1                   |
| 31  | YH    | 0                   | 1                   |
| 38  | YS    | 0                   | 1                   |
| 45  | YZ    | 0                   | 1                   |
| 48  | Y2    | 0                   | 1                   |
| 50  | R4    | 0                   | 1                   |
| 54  | R8    | 0                   | 2                   |
| 54  | Y8    | 0                   | 2                   |
| All | All   | 0                   | 13                  |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 22  | QV    | 0   | C    | OP3-P | -10.61 | 1.48        | 1.61     |
| 22  | XV    | 0   | C    | OP3-P | -10.59 | 1.48        | 1.61     |
| 35  | YP    | 63  | PRO  | N-CD  | 6.16   | 1.56        | 1.47     |
| 45  | YZ    | 159 | PRO  | N-CD  | 5.60   | 1.55        | 1.47     |
| 35  | RP    | 10  | PRO  | N-CD  | 5.58   | 1.55        | 1.47     |
| 51  | Y5    | 5   | PRO  | N-CD  | 5.52   | 1.55        | 1.47     |
| 35  | YP    | 10  | PRO  | N-CD  | 5.41   | 1.55        | 1.47     |
| 28  | YE    | 22  | PRO  | N-CD  | 5.35   | 1.55        | 1.47     |
| 45  | YZ    | 158 | PRO  | N-CD  | 5.34   | 1.55        | 1.47     |
| 51  | Y5    | 47  | PRO  | N-CD  | 5.31   | 1.55        | 1.47     |
| 31  | YH    | 154 | PRO  | N-CD  | 5.28   | 1.55        | 1.47     |
| 28  | RE    | 22  | PRO  | N-CD  | 5.15   | 1.55        | 1.47     |
| 31  | RH    | 128 | PRO  | N-CD  | 5.10   | 1.54        | 1.47     |
| 12  | XL    | 48  | PRO  | N-CD  | 5.10   | 1.54        | 1.47     |
| 29  | RF    | 25  | PRO  | N-CD  | 5.09   | 1.54        | 1.47     |
| 51  | Y5    | 7   | PRO  | N-CD  | 5.09   | 1.54        | 1.47     |

All (173) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 31  | RH    | 125 | VAL  | C-N-CD   | -17.76 | 81.53       | 120.60   |
| 25  | YA    | 771 | G    | C2-N3-C4 | -10.26 | 106.77      | 111.90   |
| 36  | RQ    | 77  | LYS  | C-N-CD   | -8.42  | 102.08      | 120.60   |
| 25  | YA    | 771 | G    | N9-C4-C5 | -8.13  | 102.15      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25  | YA    | 673  | C    | C2-N3-C4   | -7.98 | 115.91      | 119.90   |
| 26  | RB    | 95   | U    | C5-C4-O4   | 7.82  | 130.59      | 125.90   |
| 1   | QA    | 1158 | C    | C2-N1-C1'  | 7.81  | 127.39      | 118.80   |
| 1   | XA    | 1158 | C    | C2-N1-C1'  | 7.52  | 127.07      | 118.80   |
| 1   | QA    | 1495 | U    | N1-C2-O2   | 7.48  | 128.04      | 122.80   |
| 25  | RA    | 2506 | U    | C2-N1-C1'  | 7.42  | 126.61      | 117.70   |
| 26  | YB    | 81   | G    | C5-C6-O6   | -7.36 | 124.18      | 128.60   |
| 1   | QA    | 1301 | U    | C2-N1-C1'  | 7.36  | 126.53      | 117.70   |
| 1   | XA    | 1301 | U    | C2-N1-C1'  | 7.31  | 126.47      | 117.70   |
| 1   | QA    | 1158 | C    | N1-C2-O2   | 7.23  | 123.24      | 118.90   |
| 1   | XA    | 1495 | U    | N1-C2-O2   | 7.14  | 127.80      | 122.80   |
| 1   | QA    | 993  | G    | C4-N9-C1'  | 7.11  | 135.74      | 126.50   |
| 25  | YA    | 1950 | G    | N3-C4-N9   | 6.93  | 130.16      | 126.00   |
| 25  | YA    | 807  | U    | C2-N3-C4   | -6.93 | 122.84      | 127.00   |
| 25  | RA    | 2702 | U    | C2-N1-C1'  | 6.85  | 125.92      | 117.70   |
| 26  | RB    | 81   | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 25  | RA    | 828  | U    | C2-N1-C1'  | 6.80  | 125.86      | 117.70   |
| 1   | QA    | 1301 | U    | N1-C2-O2   | 6.76  | 127.53      | 122.80   |
| 25  | RA    | 673  | C    | C2-N3-C4   | -6.75 | 116.53      | 119.90   |
| 1   | QA    | 993  | G    | N3-C4-N9   | 6.70  | 130.02      | 126.00   |
| 1   | XA    | 1158 | C    | N1-C2-O2   | 6.68  | 122.91      | 118.90   |
| 1   | QA    | 1301 | U    | N3-C2-O2   | -6.64 | 117.55      | 122.20   |
| 1   | QA    | 993  | G    | C8-N9-C1'  | -6.61 | 118.41      | 127.00   |
| 4   | QD    | 28   | SER  | C-N-CD     | 6.58  | 142.23      | 128.40   |
| 25  | YA    | 1950 | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 25  | RA    | 828  | U    | N1-C2-O2   | 6.41  | 127.29      | 122.80   |
| 26  | YB    | 81   | G    | N3-C4-N9   | 6.37  | 129.82      | 126.00   |
| 1   | QA    | 754  | C    | C2-N1-C1'  | 6.35  | 125.78      | 118.80   |
| 1   | QA    | 1065 | U    | P-O3'-C3'  | 6.33  | 127.29      | 119.70   |
| 25  | YA    | 828  | U    | C2-N1-C1'  | 6.32  | 125.28      | 117.70   |
| 25  | YA    | 771  | G    | C8-N9-C4   | 6.31  | 108.92      | 106.40   |
| 26  | YB    | 81   | G    | C4-N9-C1'  | 6.31  | 134.70      | 126.50   |
| 26  | YB    | 81   | G    | C6-C5-N7   | -6.27 | 126.64      | 130.40   |
| 25  | YA    | 103  | A    | N1-C6-N6   | 6.26  | 122.36      | 118.60   |
| 25  | RA    | 807  | U    | C2-N3-C4   | -6.26 | 123.24      | 127.00   |
| 25  | YA    | 2335 | A    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |
| 25  | RA    | 828  | U    | N3-C2-O2   | -6.14 | 117.90      | 122.20   |
| 26  | YB    | 81   | G    | C8-N9-C1'  | -6.13 | 119.03      | 127.00   |
| 25  | YA    | 906  | G    | C5-C6-O6   | 6.08  | 132.25      | 128.60   |
| 1   | QA    | 1465 | C    | C2-N3-C4   | -6.07 | 116.86      | 119.90   |
| 26  | YB    | 95   | U    | C5-C4-O4   | 6.02  | 129.51      | 125.90   |
| 25  | RA    | 2335 | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25  | RA    | 669  | G    | C4-N9-C1' | 5.99  | 134.29      | 126.50   |
| 30  | RG    | 34   | LEU  | CA-CB-CG  | 5.99  | 129.08      | 115.30   |
| 41  | YV    | 35   | LEU  | CA-CB-CG  | 5.99  | 129.08      | 115.30   |
| 1   | XA    | 812  | C    | P-O3'-C3' | 5.89  | 126.77      | 119.70   |
| 29  | YF    | 74   | ARG  | NE-CZ-NH1 | 5.87  | 123.24      | 120.30   |
| 31  | YH    | 9    | ILE  | C-N-CD    | 5.87  | 140.72      | 128.40   |
| 51  | Y5    | 6    | VAL  | C-N-CD    | 5.84  | 140.66      | 128.40   |
| 25  | YA    | 103  | A    | C4-C5-C6  | 5.82  | 119.91      | 117.00   |
| 26  | YB    | 76   | G    | N3-C2-N2  | -5.82 | 115.83      | 119.90   |
| 1   | XA    | 1158 | C    | C6-N1-C2  | -5.81 | 117.98      | 120.30   |
| 28  | RE    | 63   | LEU  | CA-CB-CG  | 5.80  | 128.64      | 115.30   |
| 1   | XA    | 1301 | U    | N1-C2-O2  | 5.80  | 126.86      | 122.80   |
| 25  | YA    | 828  | U    | N1-C2-O2  | 5.77  | 126.84      | 122.80   |
| 26  | YB    | 76   | G    | C6-N1-C2  | -5.77 | 121.64      | 125.10   |
| 1   | QA    | 365  | U    | C5-C4-O4  | 5.76  | 129.36      | 125.90   |
| 29  | RF    | 24   | LEU  | C-N-CD    | 5.73  | 140.43      | 128.40   |
| 25  | YA    | 1130 | U    | P-O3'-C3' | 5.70  | 126.54      | 119.70   |
| 51  | Y5    | 46   | CYS  | C-N-CD    | 5.69  | 140.35      | 128.40   |
| 1   | QA    | 49   | U    | C5-C4-O4  | 5.69  | 129.31      | 125.90   |
| 25  | RA    | 2702 | U    | C5-C6-N1  | 5.68  | 125.54      | 122.70   |
| 31  | RH    | 127  | GLU  | C-N-CD    | 5.67  | 140.31      | 128.40   |
| 25  | YA    | 2506 | U    | C2-N1-C1' | 5.67  | 124.50      | 117.70   |
| 25  | YA    | 669  | G    | C4-N9-C1' | 5.66  | 133.86      | 126.50   |
| 1   | QA    | 1158 | C    | N3-C2-O2  | -5.66 | 117.94      | 121.90   |
| 35  | YP    | 59   | LEU  | CA-CB-CG  | 5.66  | 128.31      | 115.30   |
| 26  | RB    | 76   | G    | C6-N1-C2  | -5.65 | 121.71      | 125.10   |
| 1   | QA    | 1065 | U    | OP2-P-O3' | 5.62  | 117.56      | 105.20   |
| 12  | XL    | 47   | LYS  | C-N-CD    | 5.59  | 140.15      | 128.40   |
| 35  | YP    | 10   | PRO  | CA-N-CD   | -5.58 | 103.68      | 111.50   |
| 1   | QA    | 1158 | C    | C6-N1-C2  | -5.58 | 118.07      | 120.30   |
| 25  | YA    | 673  | C    | N3-C4-C5  | 5.58  | 124.13      | 121.90   |
| 25  | YA    | 2447 | G    | C6-N1-C2  | -5.58 | 121.75      | 125.10   |
| 28  | RE    | 22   | PRO  | CA-N-CD   | -5.56 | 103.71      | 111.50   |
| 27  | YD    | 229  | VAL  | CB-CA-C   | -5.56 | 100.84      | 111.40   |
| 25  | YA    | 828  | U    | N3-C2-O2  | -5.56 | 118.31      | 122.20   |
| 1   | XA    | 1158 | C    | N3-C2-O2  | -5.55 | 118.01      | 121.90   |
| 25  | YA    | 771  | G    | C4-C5-N7  | 5.53  | 113.01      | 110.80   |
| 1   | QA    | 993  | G    | C6-C5-N7  | -5.52 | 127.09      | 130.40   |
| 25  | YA    | 99   | U    | P-O3'-C3' | 5.52  | 126.32      | 119.70   |
| 1   | XA    | 410  | G    | OP1-P-O3' | 5.51  | 117.33      | 105.20   |
| 31  | YH    | 153  | LYS  | C-N-CD    | 5.51  | 139.98      | 128.40   |
| 25  | RA    | 103  | A    | N1-C6-N6  | 5.51  | 121.91      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 28  | YE    | 21   | VAL  | C-N-CD     | 5.50  | 139.96      | 128.40   |
| 1   | QA    | 1046 | A    | C5-C6-N1   | 5.50  | 120.45      | 117.70   |
| 25  | RA    | 2447 | G    | C6-N1-C2   | -5.50 | 121.80      | 125.10   |
| 1   | QA    | 993  | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | XA    | 328  | C    | N1-C2-O2   | 5.48  | 122.19      | 118.90   |
| 1   | QA    | 49   | U    | N3-C4-O4   | -5.46 | 115.58      | 119.40   |
| 28  | RE    | 27   | LEU  | CA-CB-CG   | 5.46  | 127.87      | 115.30   |
| 25  | YA    | 771  | G    | N3-C4-C5   | 5.46  | 131.33      | 128.60   |
| 35  | RP    | 88   | LEU  | CA-CB-CG   | 5.46  | 127.85      | 115.30   |
| 1   | QA    | 1027 | C    | OP1-P-O3'  | 5.44  | 117.18      | 105.20   |
| 1   | XA    | 328  | C    | C2-N1-C1'  | 5.44  | 124.78      | 118.80   |
| 25  | YA    | 99   | U    | OP2-P-O3'  | 5.41  | 117.10      | 105.20   |
| 12  | XL    | 47   | LYS  | N-CA-C     | 5.39  | 125.56      | 111.00   |
| 1   | XA    | 812  | C    | OP2-P-O3'  | 5.38  | 117.04      | 105.20   |
| 1   | XA    | 1301 | U    | N3-C2-O2   | -5.38 | 118.43      | 122.20   |
| 25  | YA    | 1313 | U    | C2-N1-C1'  | 5.38  | 124.16      | 117.70   |
| 25  | RA    | 673  | C    | C5-C4-N4   | -5.37 | 116.44      | 120.20   |
| 25  | YA    | 1950 | G    | C8-N9-C1'  | -5.37 | 120.02      | 127.00   |
| 26  | YB    | 100  | G    | C8-N9-C1'  | 5.37  | 133.97      | 127.00   |
| 45  | YZ    | 115  | GLY  | N-CA-C     | -5.36 | 99.71       | 113.10   |
| 26  | RB    | 76   | G    | N3-C2-N2   | -5.35 | 116.16      | 119.90   |
| 25  | RA    | 669  | G    | C8-N9-C1'  | -5.34 | 120.06      | 127.00   |
| 25  | RA    | 205  | G    | P-O3'-C3'  | 5.33  | 126.10      | 119.70   |
| 25  | RA    | 404  | C    | P-O3'-C3'  | 5.33  | 126.10      | 119.70   |
| 1   | QA    | 701  | C    | OP2-P-O3'  | 5.32  | 116.90      | 105.20   |
| 45  | YZ    | 158  | PRO  | C-N-CD     | 5.32  | 139.57      | 128.40   |
| 35  | YP    | 25   | SER  | N-CA-C     | -5.29 | 96.71       | 111.00   |
| 18  | QR    | 31   | LEU  | CA-CB-CG   | 5.29  | 127.47      | 115.30   |
| 26  | RB    | 31   | C    | N1-C2-O2   | 5.29  | 122.07      | 118.90   |
| 45  | YZ    | 157  | LEU  | C-N-CD     | 5.27  | 139.46      | 128.40   |
| 1   | QA    | 328  | C    | P-O3'-C3'  | 5.26  | 126.01      | 119.70   |
| 25  | YA    | 503  | A    | P-O3'-C3'  | 5.26  | 126.01      | 119.70   |
| 25  | YA    | 2378 | A    | N1-C6-N6   | 5.26  | 121.75      | 118.60   |
| 1   | XA    | 1027 | C    | OP1-P-O3'  | 5.25  | 116.76      | 105.20   |
| 1   | QA    | 1158 | C    | C6-N1-C1'  | -5.25 | 114.50      | 120.80   |
| 35  | YP    | 62   | LEU  | C-N-CD     | 5.24  | 139.41      | 128.40   |
| 25  | YA    | 1950 | G    | C4-N9-C1'  | 5.23  | 133.30      | 126.50   |
| 1   | QA    | 1027 | C    | P-O3'-C3'  | 5.23  | 125.98      | 119.70   |
| 26  | RB    | 81   | G    | C6-N1-C2   | -5.23 | 121.96      | 125.10   |
| 25  | RA    | 103  | A    | C4-C5-C6   | 5.22  | 119.61      | 117.00   |
| 25  | YA    | 1779 | U    | C2-N1-C1'  | 5.22  | 123.96      | 117.70   |
| 34  | RO    | 8    | LEU  | CA-CB-CG   | 5.21  | 127.28      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25  | RA    | 2506 | U    | C6-N1-C1'  | -5.20 | 113.92      | 121.20   |
| 22  | XV    | 16   | C    | C2-N1-C1'  | 5.19  | 124.50      | 118.80   |
| 19  | XS    | 41   | VAL  | C-N-CD     | -5.18 | 109.20      | 120.60   |
| 25  | RA    | 2702 | U    | N1-C2-O2   | 5.17  | 126.42      | 122.80   |
| 26  | RB    | 81   | G    | N3-C4-N9   | 5.17  | 129.10      | 126.00   |
| 25  | YA    | 1372 | U    | C5-C4-O4   | -5.16 | 122.81      | 125.90   |
| 25  | RA    | 1312 | U    | P-O3'-C3'  | 5.16  | 125.89      | 119.70   |
| 25  | RA    | 1535 | U    | C2-N1-C1'  | 5.15  | 123.88      | 117.70   |
| 26  | YB    | 81   | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | XA    | 1465 | C    | C2-N3-C4   | -5.14 | 117.33      | 119.90   |
| 1   | QA    | 754  | C    | N1-C2-O2   | 5.14  | 121.98      | 118.90   |
| 1   | QA    | 1436 | U    | C2-N3-C4   | -5.14 | 123.92      | 127.00   |
| 1   | QA    | 1322 | C    | C2-N1-C1'  | 5.13  | 124.45      | 118.80   |
| 25  | RA    | 1799 | G    | P-O3'-C3'  | 5.13  | 125.86      | 119.70   |
| 25  | RA    | 1992 | G    | P-O3'-C3'  | 5.12  | 125.85      | 119.70   |
| 26  | YB    | 81   | G    | N1-C6-O6   | 5.11  | 122.97      | 119.90   |
| 1   | QA    | 1297 | C    | P-O3'-C3'  | 5.11  | 125.83      | 119.70   |
| 25  | YA    | 2832 | U    | P-O3'-C3'  | 5.11  | 125.83      | 119.70   |
| 25  | YA    | 222  | A    | P-O3'-C3'  | 5.10  | 125.82      | 119.70   |
| 25  | YA    | 2053 | G    | C5-N7-C8   | -5.10 | 101.75      | 104.30   |
| 25  | RA    | 2726 | U    | C2-N1-C1'  | 5.09  | 123.81      | 117.70   |
| 1   | XA    | 1297 | C    | P-O3'-C3'  | 5.09  | 125.81      | 119.70   |
| 25  | YA    | 669  | G    | C8-N9-C1'  | -5.09 | 120.38      | 127.00   |
| 25  | YA    | 1396 | U    | N1-C2-O2   | 5.09  | 126.36      | 122.80   |
| 41  | RV    | 35   | LEU  | CA-CB-CG   | 5.09  | 127.00      | 115.30   |
| 25  | RA    | 2506 | U    | N1-C2-O2   | 5.08  | 126.36      | 122.80   |
| 1   | XA    | 328  | C    | P-O3'-C3'  | 5.08  | 125.80      | 119.70   |
| 25  | YA    | 807  | U    | C5-C4-O4   | -5.05 | 122.87      | 125.90   |
| 25  | RA    | 537  | C    | C2-N1-C1'  | 5.05  | 124.36      | 118.80   |
| 25  | YA    | 1141 | U    | C2-N3-C4   | -5.05 | 123.97      | 127.00   |
| 25  | YA    | 1992 | G    | P-O3'-C3'  | 5.04  | 125.75      | 119.70   |
| 28  | YE    | 117  | MET  | CA-CB-CG   | 5.04  | 121.87      | 113.30   |
| 51  | Y5    | 4    | HIS  | C-N-CD     | 5.03  | 138.97      | 128.40   |
| 25  | RA    | 242  | G    | P-O3'-C3'  | 5.03  | 125.74      | 119.70   |
| 25  | YA    | 404  | C    | P-O3'-C3'  | 5.03  | 125.74      | 119.70   |
| 45  | YZ    | 150  | LEU  | CA-CB-CG   | 5.03  | 126.86      | 115.30   |
| 1   | XA    | 1436 | U    | C2-N3-C4   | -5.03 | 123.98      | 127.00   |
| 25  | YA    | 2681 | C    | P-O3'-C3'  | 5.02  | 125.73      | 119.70   |
| 1   | QA    | 992  | U    | P-O3'-C3'  | 5.02  | 125.72      | 119.70   |
| 1   | QA    | 1465 | C    | C5-C4-N4   | -5.01 | 116.69      | 120.20   |
| 32  | RI    | 74   | ASN  | N-CA-C     | 5.01  | 124.54      | 111.00   |
| 25  | YA    | 1558 | A    | P-O3'-C3'  | 5.01  | 125.71      | 119.70   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 25  | RA    | 222 | A    | P-O3'-C3' | 5.00 | 125.70      | 119.70   |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 12  | QL    | 47  | LYS  | Peptide   |
| 50  | R4    | 38  | LYS  | Peptide   |
| 54  | R8    | 30  | ARG  | Peptide   |
| 54  | R8    | 35  | GLN  | Peptide   |
| 31  | RH    | 153 | LYS  | Peptide   |
| 12  | XL    | 12  | ARG  | Sidechain |
| 48  | Y2    | 17  | SER  | Peptide   |
| 54  | Y8    | 30  | ARG  | Peptide   |
| 54  | Y8    | 51  | ALA  | Peptide   |
| 29  | YF    | 47  | GLY  | Peptide   |
| 31  | YH    | 127 | GLU  | Peptide   |
| 38  | YS    | 109 | GLY  | Peptide   |
| 45  | YZ    | 181 | GLU  | 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   | QA    | 32247 | 0        | 16278    | 479     | 0            |
| 1   | XA    | 32249 | 0        | 16279    | 433     | 0            |
| 2   | QB    | 1924  | 0        | 1975     | 62      | 0            |
| 2   | XB    | 1924  | 0        | 1975     | 83      | 0            |
| 3   | QC    | 1605  | 0        | 1668     | 49      | 0            |
| 3   | XC    | 1605  | 0        | 1668     | 57      | 0            |
| 4   | QD    | 1703  | 0        | 1763     | 93      | 0            |
| 4   | XD    | 1703  | 0        | 1765     | 50      | 1            |
| 5   | QE    | 1155  | 0        | 1213     | 28      | 0            |
| 5   | XE    | 1155  | 0        | 1213     | 42      | 0            |
| 6   | QF    | 843   | 0        | 857      | 29      | 0            |
| 6   | XF    | 843   | 0        | 857      | 40      | 0            |
| 7   | QG    | 1257  | 0        | 1296     | 46      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | XG    | 1257  | 0        | 1296     | 24      | 0            |
| 8   | QH    | 1116  | 0        | 1175     | 38      | 0            |
| 8   | XH    | 1116  | 0        | 1177     | 28      | 0            |
| 9   | QI    | 1010  | 0        | 1037     | 37      | 0            |
| 9   | XI    | 1010  | 0        | 1037     | 49      | 0            |
| 10  | QJ    | 801   | 0        | 849      | 51      | 0            |
| 10  | XJ    | 801   | 0        | 849      | 42      | 0            |
| 11  | QK    | 885   | 0        | 904      | 36      | 0            |
| 11  | XK    | 885   | 0        | 904      | 37      | 0            |
| 12  | QL    | 975   | 0        | 1062     | 39      | 0            |
| 12  | XL    | 975   | 0        | 1062     | 50      | 0            |
| 13  | QM    | 964   | 0        | 1034     | 64      | 0            |
| 13  | XM    | 964   | 0        | 1034     | 61      | 0            |
| 14  | QN    | 492   | 0        | 529      | 27      | 0            |
| 14  | XN    | 492   | 0        | 529      | 18      | 0            |
| 15  | QO    | 734   | 0        | 771      | 20      | 0            |
| 15  | XO    | 734   | 0        | 771      | 18      | 0            |
| 16  | QP    | 705   | 0        | 725      | 16      | 0            |
| 16  | XP    | 705   | 0        | 725      | 25      | 0            |
| 17  | QQ    | 834   | 0        | 904      | 23      | 0            |
| 17  | XQ    | 834   | 0        | 904      | 14      | 0            |
| 18  | QR    | 574   | 0        | 644      | 10      | 0            |
| 18  | XR    | 574   | 0        | 644      | 25      | 0            |
| 19  | QS    | 674   | 0        | 699      | 74      | 0            |
| 19  | XS    | 674   | 0        | 699      | 74      | 0            |
| 20  | QT    | 763   | 0        | 861      | 20      | 0            |
| 20  | XT    | 763   | 0        | 861      | 35      | 0            |
| 21  | QU    | 217   | 0        | 234      | 11      | 0            |
| 21  | XU    | 217   | 0        | 234      | 2       | 0            |
| 22  | QV    | 1644  | 0        | 835      | 17      | 0            |
| 22  | XV    | 1644  | 0        | 836      | 18      | 0            |
| 23  | QW    | 1619  | 0        | 822      | 25      | 0            |
| 23  | QY    | 364   | 0        | 186      | 2       | 0            |
| 23  | XW    | 1619  | 0        | 822      | 30      | 0            |
| 23  | XY    | 364   | 0        | 186      | 2       | 0            |
| 24  | QX    | 210   | 0        | 109      | 0       | 0            |
| 24  | XX    | 210   | 0        | 109      | 1       | 0            |
| 25  | RA    | 62071 | 0        | 31284    | 759     | 1            |
| 25  | YA    | 62091 | 0        | 31294    | 730     | 0            |
| 26  | RB    | 2573  | 0        | 1306     | 41      | 0            |
| 26  | YB    | 2573  | 0        | 1306     | 34      | 0            |
| 27  | RD    | 2115  | 0        | 2195     | 95      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27  | YD    | 2115  | 0        | 2195     | 139     | 0            |
| 28  | RE    | 1568  | 0        | 1634     | 92      | 0            |
| 28  | YE    | 1568  | 0        | 1634     | 72      | 0            |
| 29  | RF    | 1585  | 0        | 1632     | 85      | 0            |
| 29  | YF    | 1585  | 0        | 1632     | 62      | 0            |
| 30  | RG    | 1474  | 0        | 1535     | 65      | 0            |
| 30  | YG    | 1474  | 0        | 1535     | 62      | 0            |
| 31  | RH    | 1307  | 0        | 1382     | 74      | 0            |
| 31  | YH    | 1307  | 0        | 1382     | 89      | 0            |
| 32  | RI    | 1136  | 0        | 1223     | 75      | 0            |
| 32  | YI    | 1136  | 0        | 1223     | 52      | 0            |
| 33  | RN    | 1104  | 0        | 1180     | 41      | 0            |
| 33  | YN    | 1104  | 0        | 1180     | 50      | 0            |
| 34  | RO    | 933   | 0        | 996      | 23      | 0            |
| 34  | YO    | 933   | 0        | 996      | 21      | 0            |
| 35  | RP    | 1145  | 0        | 1226     | 82      | 0            |
| 35  | YP    | 1145  | 0        | 1228     | 88      | 0            |
| 36  | RQ    | 1122  | 0        | 1179     | 57      | 0            |
| 36  | YQ    | 1122  | 0        | 1178     | 50      | 0            |
| 37  | RR    | 968   | 0        | 1033     | 49      | 0            |
| 37  | YR    | 968   | 0        | 1033     | 35      | 0            |
| 38  | RS    | 882   | 0        | 943      | 42      | 0            |
| 38  | YS    | 882   | 0        | 943      | 45      | 0            |
| 39  | RT    | 1141  | 0        | 1202     | 63      | 0            |
| 39  | YT    | 1141  | 0        | 1202     | 53      | 0            |
| 40  | RU    | 964   | 0        | 1022     | 31      | 0            |
| 40  | YU    | 964   | 0        | 1022     | 52      | 0            |
| 41  | RV    | 779   | 0        | 852      | 20      | 0            |
| 41  | YV    | 779   | 0        | 852      | 43      | 0            |
| 42  | RW    | 900   | 0        | 964      | 24      | 0            |
| 42  | YW    | 900   | 0        | 964      | 27      | 0            |
| 43  | RX    | 725   | 0        | 778      | 29      | 0            |
| 43  | YX    | 725   | 0        | 778      | 23      | 0            |
| 44  | RY    | 785   | 0        | 878      | 48      | 0            |
| 44  | YY    | 785   | 0        | 878      | 40      | 0            |
| 45  | RZ    | 1461  | 0        | 1493     | 64      | 0            |
| 45  | YZ    | 1461  | 0        | 1493     | 80      | 0            |
| 46  | R0    | 648   | 0        | 672      | 21      | 0            |
| 46  | Y0    | 648   | 0        | 672      | 31      | 0            |
| 47  | R1    | 763   | 0        | 848      | 29      | 0            |
| 47  | Y1    | 763   | 0        | 848      | 28      | 0            |
| 48  | R2    | 581   | 0        | 629      | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | Y2    | 581   | 0        | 629      | 23      | 0            |
| 49  | R3    | 469   | 0        | 518      | 6       | 0            |
| 49  | Y3    | 469   | 0        | 518      | 15      | 0            |
| 50  | R4    | 581   | 0        | 574      | 77      | 0            |
| 50  | Y4    | 581   | 0        | 574      | 98      | 0            |
| 51  | R5    | 459   | 0        | 476      | 68      | 0            |
| 51  | Y5    | 442   | 0        | 465      | 35      | 0            |
| 52  | R6    | 424   | 0        | 450      | 26      | 0            |
| 52  | Y6    | 424   | 0        | 450      | 32      | 0            |
| 53  | R7    | 430   | 0        | 480      | 20      | 0            |
| 53  | Y7    | 430   | 0        | 480      | 15      | 0            |
| 54  | R8    | 517   | 0        | 582      | 30      | 0            |
| 54  | Y8    | 517   | 0        | 582      | 40      | 0            |
| 55  | R9    | 307   | 0        | 338      | 8       | 0            |
| 55  | Y9    | 307   | 0        | 336      | 8       | 0            |
| 56  | Z7    | 116   | 0        | 134      | 13      | 0            |
| 56  | Z8    | 116   | 0        | 133      | 5       | 0            |
| 57  | QA    | 67    | 0        | 0        | 0       | 0            |
| 57  | QF    | 1     | 0        | 0        | 0       | 0            |
| 57  | QH    | 1     | 0        | 0        | 0       | 0            |
| 57  | QV    | 2     | 0        | 0        | 0       | 0            |
| 57  | QY    | 1     | 0        | 0        | 0       | 0            |
| 57  | R0    | 1     | 0        | 0        | 0       | 0            |
| 57  | R5    | 1     | 0        | 0        | 0       | 0            |
| 57  | RA    | 246   | 0        | 0        | 0       | 0            |
| 57  | RB    | 2     | 0        | 0        | 0       | 0            |
| 57  | RD    | 1     | 0        | 0        | 0       | 0            |
| 57  | RE    | 1     | 0        | 0        | 0       | 0            |
| 57  | RP    | 4     | 0        | 0        | 0       | 0            |
| 57  | XA    | 71    | 0        | 0        | 0       | 0            |
| 57  | XB    | 1     | 0        | 0        | 0       | 0            |
| 57  | XM    | 1     | 0        | 0        | 0       | 0            |
| 57  | XV    | 3     | 0        | 0        | 0       | 0            |
| 57  | XX    | 1     | 0        | 0        | 0       | 0            |
| 57  | XY    | 1     | 0        | 0        | 0       | 0            |
| 57  | Y5    | 1     | 0        | 0        | 0       | 0            |
| 57  | Y7    | 1     | 0        | 0        | 0       | 0            |
| 57  | YA    | 278   | 0        | 0        | 0       | 0            |
| 57  | YB    | 5     | 0        | 0        | 0       | 0            |
| 57  | YD    | 1     | 0        | 0        | 0       | 0            |
| 57  | YE    | 2     | 0        | 0        | 0       | 0            |
| 57  | YP    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | YX    | 1      | 0        | 0        | 0       | 0            |
| 58  | QA    | 42     | 0        | 45       | 1       | 0            |
| 58  | XA    | 42     | 0        | 45       | 4       | 0            |
| 59  | QD    | 1      | 0        | 0        | 0       | 0            |
| 59  | QN    | 1      | 0        | 0        | 0       | 0            |
| 59  | R5    | 1      | 0        | 0        | 0       | 0            |
| 59  | XD    | 1      | 0        | 0        | 0       | 0            |
| 59  | XN    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y9    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 295487 | 0        | 200229   | 5889    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (5889) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:YQ:134:ARG:CZ   | 45:YZ:122:ARG:HH21 | 1.34                     | 1.39              |
| 28:YE:14:ILE:HG22  | 28:YE:21:VAL:CG2   | 1.56                     | 1.35              |
| 27:YD:121:PRO:HB3  | 27:YD:135:PHE:CE2  | 1.64                     | 1.31              |
| 28:YE:14:ILE:CG2   | 28:YE:21:VAL:HG23  | 1.62                     | 1.29              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CD   | 1.64                     | 1.25              |
| 45:YZ:93:ASP:O     | 45:YZ:94:GLU:HG2   | 1.10                     | 1.24              |
| 28:RE:21:VAL:HG23  | 28:RE:22:PRO:CB    | 1.69                     | 1.22              |
| 27:YD:121:PRO:CB   | 27:YD:135:PHE:HE2  | 1.55                     | 1.18              |
| 4:QD:167:GLY:HA3   | 27:YD:135:PHE:HE1  | 1.10                     | 1.17              |
| 13:QM:80:ARG:HD3   | 50:R4:71:ARG:NH2   | 1.59                     | 1.17              |
| 51:Y5:46:CYS:SG    | 51:Y5:50:GLY:HA3   | 1.84                     | 1.16              |
| 31:RH:125:VAL:CG1  | 31:RH:126:PRO:HD3  | 1.75                     | 1.16              |
| 19:XS:42:PRO:HB3   | 50:Y4:60:GLN:OE1   | 1.49                     | 1.13              |
| 4:XD:22:LYS:HD3    | 4:XD:26:CYS:SG     | 1.89                     | 1.12              |
| 4:QD:166:LYS:HG3   | 4:QD:178:VAL:HG11  | 1.32                     | 1.10              |
| 25:RA:1169:G:H1    | 25:RA:1180:C:N4    | 1.48                     | 1.09              |
| 28:RE:21:VAL:HG23  | 28:RE:22:PRO:HB3   | 1.18                     | 1.09              |
| 27:YD:121:PRO:CB   | 27:YD:135:PHE:CE2  | 2.34                     | 1.09              |
| 36:YQ:134:ARG:CZ   | 45:YZ:122:ARG:NH2  | 2.16                     | 1.09              |
| 32:YI:53:ALA:O     | 32:YI:57:ARG:HG3   | 1.52                     | 1.08              |
| 25:YA:1169:G:H1    | 25:YA:1180:C:N4    | 1.52                     | 1.07              |
| 31:YH:10:PRO:HG2   | 31:YH:50:VAL:HG13  | 1.32                     | 1.06              |
| 4:QD:167:GLY:CA    | 27:YD:135:PHE:CE1  | 2.39                     | 1.05              |
| 4:QD:167:GLY:HA3   | 27:YD:135:PHE:CE1  | 1.90                     | 1.05              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:93:ASP:O     | 45:YZ:94:GLU:CG    | 2.03                     | 1.05              |
| 28:RE:21:VAL:CG2   | 28:RE:22:PRO:HB3   | 1.87                     | 1.05              |
| 51:R5:50:GLY:HA3   | 51:R5:56:LYS:HB3   | 1.38                     | 1.04              |
| 51:Y5:46:CYS:SG    | 51:Y5:50:GLY:CA    | 2.44                     | 1.04              |
| 53:R7:9:ARG:HH21   | 53:R7:48:LYS:HD2   | 1.16                     | 1.04              |
| 45:YZ:91:LEU:HG    | 45:YZ:130:PRO:HB3  | 1.41                     | 1.03              |
| 25:YA:1359:A:N6    | 25:YA:1372:U:N3    | 2.07                     | 1.02              |
| 32:RI:52:ARG:O     | 32:RI:56:LYS:N     | 1.91                     | 1.02              |
| 28:YE:24:THR:HG21  | 28:YE:188:VAL:HG11 | 1.37                     | 1.02              |
| 4:QD:28:SER:HB3    | 4:QD:29:PRO:HD3    | 1.39                     | 1.00              |
| 19:QS:67:VAL:HB    | 50:R4:59:PHE:CE2   | 1.96                     | 1.00              |
| 19:QS:67:VAL:HG12  | 50:R4:59:PHE:CE1   | 1.96                     | 0.99              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:HD3  | 1.01                     | 0.99              |
| 31:YH:10:PRO:CG    | 31:YH:50:VAL:HG13  | 1.91                     | 0.99              |
| 25:RA:1542:G:H3'   | 25:RA:1543:A:C5'   | 1.92                     | 0.99              |
| 6:XF:100:ASN:O     | 18:XR:28:GLU:HG2   | 1.61                     | 0.98              |
| 25:YA:2099:U:H3    | 25:YA:2190:G:H1    | 1.05                     | 0.98              |
| 25:YA:2287:A:H62   | 25:YA:2344:U:H3    | 1.04                     | 0.98              |
| 4:XD:22:LYS:CD     | 4:XD:26:CYS:SG     | 2.52                     | 0.98              |
| 28:YE:14:ILE:CG2   | 28:YE:21:VAL:CG2   | 2.29                     | 0.98              |
| 51:R5:58:LEU:HD13  | 51:R5:60:VAL:HG12  | 1.41                     | 0.97              |
| 13:XM:54:VAL:HG23  | 50:Y4:32:TYR:OH    | 1.64                     | 0.97              |
| 4:QD:9:CYS:SG      | 4:QD:22:LYS:CE     | 2.52                     | 0.97              |
| 13:QM:7:VAL:HG21   | 30:RG:113:ARG:O    | 1.63                     | 0.97              |
| 25:YA:2701:C:H3'   | 25:YA:2702:U:H5''  | 1.43                     | 0.97              |
| 38:YS:59:LYS:HD3   | 38:YS:60:GLY:N     | 1.80                     | 0.97              |
| 25:RA:1542:G:H3'   | 25:RA:1543:A:H5'   | 1.43                     | 0.96              |
| 13:QM:80:ARG:HE    | 50:R4:71:ARG:HH12  | 1.08                     | 0.96              |
| 25:RA:2053:G:O6    | 25:RA:2614:A:H2    | 1.49                     | 0.96              |
| 1:XA:963:G:H1      | 1:XA:972:C:H42     | 1.09                     | 0.96              |
| 28:YE:24:THR:HG21  | 28:YE:188:VAL:CG1  | 1.97                     | 0.95              |
| 4:QD:167:GLY:HA2   | 27:YD:135:PHE:CZ   | 2.01                     | 0.95              |
| 28:RE:20:ALA:O     | 28:RE:21:VAL:HG13  | 1.65                     | 0.95              |
| 28:RE:13:ARG:HB2   | 28:RE:21:VAL:HG12  | 1.47                     | 0.95              |
| 4:QD:9:CYS:SG      | 4:QD:22:LYS:HE3    | 2.07                     | 0.95              |
| 19:QS:67:VAL:HB    | 50:R4:59:PHE:CZ    | 2.01                     | 0.94              |
| 29:YF:68:LYS:HG2   | 29:YF:69:HIS:CE1   | 2.02                     | 0.94              |
| 27:YD:121:PRO:CA   | 27:YD:135:PHE:CE2  | 2.50                     | 0.94              |
| 29:YF:68:LYS:HG2   | 29:YF:69:HIS:ND1   | 1.83                     | 0.94              |
| 25:YA:896:A:H1'    | 45:YZ:176:PRO:HB3  | 1.50                     | 0.94              |
| 19:QS:70:LYS:CE    | 50:R4:68:ARG:HH21  | 1.79                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:95:PRO:HG2   | 45:YZ:127:LYS:HD3  | 1.48                     | 0.94              |
| 12:XL:48:PRO:O     | 12:XL:49:ASN:ND2   | 2.00                     | 0.93              |
| 19:QS:70:LYS:HE2   | 50:R4:68:ARG:NH2   | 1.83                     | 0.93              |
| 25:YA:1533:C:H42   | 25:YA:1538:G:H1    | 1.01                     | 0.93              |
| 2:QB:185:ILE:HG22  | 2:QB:199:TYR:HB2   | 1.48                     | 0.93              |
| 27:YD:121:PRO:HA   | 27:YD:135:PHE:CE2  | 2.03                     | 0.93              |
| 1:QA:1002:G:H1     | 1:QA:1038:C:H42    | 1.00                     | 0.93              |
| 32:RI:57:ARG:O     | 32:RI:61:ARG:HG2   | 1.67                     | 0.93              |
| 51:R5:55:ARG:NH1   | 51:R5:57:VAL:HA    | 1.83                     | 0.93              |
| 25:RA:2308:G:H1    | 25:RA:2311:A:H2    | 1.15                     | 0.93              |
| 28:RE:21:VAL:HG23  | 28:RE:22:PRO:CA    | 1.99                     | 0.92              |
| 32:RI:52:ARG:HB2   | 32:RI:56:LYS:HB2   | 1.48                     | 0.92              |
| 1:XA:954:G:H21     | 1:XA:1227:A:H62    | 1.01                     | 0.92              |
| 27:YD:121:PRO:CA   | 27:YD:135:PHE:HE2  | 1.82                     | 0.92              |
| 26:RB:38:C:H42     | 26:RB:44:G:H1      | 1.17                     | 0.92              |
| 27:YD:121:PRO:HA   | 27:YD:135:PHE:CD2  | 2.05                     | 0.92              |
| 32:RI:52:ARG:O     | 32:RI:56:LYS:HB3   | 1.69                     | 0.92              |
| 51:Y5:33:CYS:HG    | 51:Y5:46:CYS:HG    | 1.17                     | 0.92              |
| 1:XA:963:G:N2      | 1:XA:972:C:N3      | 2.18                     | 0.91              |
| 38:YS:59:LYS:HD3   | 38:YS:60:GLY:H     | 1.34                     | 0.91              |
| 35:RP:58:THR:O     | 35:RP:61:ARG:NE    | 2.03                     | 0.91              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CG   | 1.98                     | 0.91              |
| 19:XS:67:VAL:HG21  | 50:Y4:60:GLN:HE22  | 1.32                     | 0.91              |
| 25:YA:49:A:N7      | 25:YA:120:U:C4     | 2.38                     | 0.91              |
| 32:YI:52:ARG:O     | 32:YI:56:LYS:HB3   | 1.71                     | 0.91              |
| 25:YA:993:G:OP1    | 40:YU:50:ARG:NH2   | 2.04                     | 0.91              |
| 25:RA:1043:C:H42   | 25:RA:1112:G:H1    | 0.97                     | 0.91              |
| 13:QM:80:ARG:HD3   | 50:R4:71:ARG:HH22  | 1.33                     | 0.90              |
| 51:R5:40:LYS:NZ    | 51:R5:46:CYS:SG    | 2.45                     | 0.90              |
| 25:YA:1338:G:N7    | 43:YX:62:LYS:NZ    | 2.20                     | 0.90              |
| 4:QD:28:SER:HB3    | 4:QD:29:PRO:CD     | 1.96                     | 0.90              |
| 45:YZ:151:HIS:HB3  | 45:YZ:170:THR:HA   | 1.54                     | 0.90              |
| 25:RA:2580:U:H4'   | 28:RE:130:GLY:HA3  | 1.54                     | 0.90              |
| 36:RQ:81:VAL:O     | 36:RQ:82:ARG:NE    | 2.05                     | 0.89              |
| 1:XA:954:G:N2      | 1:XA:1227:A:H62    | 1.70                     | 0.89              |
| 25:YA:1359:A:N6    | 25:YA:1372:U:H3    | 1.71                     | 0.89              |
| 32:RI:54:GLN:O     | 32:RI:58:LEU:HB2   | 1.73                     | 0.89              |
| 25:RA:2839:G:H5'   | 37:RR:46:GLY:HA2   | 1.54                     | 0.89              |
| 28:YE:50:GLY:HA2   | 28:YE:77:ILE:HA    | 1.53                     | 0.89              |
| 19:QS:70:LYS:NZ    | 50:R4:68:ARG:HH21  | 1.70                     | 0.89              |
| 36:YQ:134:ARG:NH1  | 45:YZ:122:ARG:HH21 | 1.69                     | 0.89              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:QS:70:LYS:HE2   | 50:R4:68:ARG:HH21 | 1.34                     | 0.89              |
| 1:QA:49:U:C4       | 1:QA:365:U:O4     | 2.26                     | 0.88              |
| 39:RT:26:ASP:HB3   | 39:RT:92:GLY:H    | 1.36                     | 0.88              |
| 51:R5:49:CYS:O     | 51:R5:56:LYS:HD2  | 1.73                     | 0.88              |
| 25:RA:2287:A:N6    | 25:RA:2344:U:H3   | 1.71                     | 0.88              |
| 44:YY:79:CYS:SG    | 44:YY:80:GLY:N    | 2.45                     | 0.88              |
| 13:XM:68:GLY:HA3   | 30:YG:116:ASP:OD1 | 1.73                     | 0.88              |
| 25:RA:2701:C:H3'   | 25:RA:2702:U:H5'' | 1.52                     | 0.88              |
| 1:QA:963:G:H1      | 1:QA:972:C:H42    | 1.22                     | 0.88              |
| 51:R5:55:ARG:HG3   | 51:R5:57:VAL:H    | 1.37                     | 0.88              |
| 1:XA:1008:C:H42    | 1:XA:1021:G:H1    | 1.17                     | 0.88              |
| 31:YH:152:ARG:HG3  | 31:YH:153:LYS:HD2 | 1.53                     | 0.88              |
| 29:RF:6:VAL:HB     | 29:RF:24:LEU:HB2  | 1.57                     | 0.87              |
| 31:YH:10:PRO:HD3   | 31:YH:50:VAL:O    | 1.73                     | 0.87              |
| 28:RE:13:ARG:HB2   | 28:RE:21:VAL:CG1  | 2.03                     | 0.87              |
| 31:YH:109:PHE:CZ   | 31:YH:152:ARG:HD3 | 2.09                     | 0.87              |
| 51:R5:49:CYS:O     | 51:R5:56:LYS:CD   | 2.22                     | 0.87              |
| 35:RP:64:LYS:O     | 35:RP:66:GLY:N    | 2.07                     | 0.87              |
| 25:YA:847:U:O4     | 25:YA:933:A:N1    | 2.08                     | 0.87              |
| 44:YY:76:CYS:HB3   | 44:YY:96:ILE:HD13 | 1.57                     | 0.87              |
| 1:QA:49:U:C5       | 1:QA:365:U:O4     | 2.27                     | 0.87              |
| 56:Z8:1:T17:H10    | 56:Z8:1:T17:H55   | 1.54                     | 0.87              |
| 25:RA:1543:A:H1'   | 25:RA:1545:A:O4'  | 1.75                     | 0.87              |
| 3:QC:79:ARG:HD2    | 11:XK:99:GLN:NE2  | 1.88                     | 0.87              |
| 13:XM:54:VAL:CG2   | 50:Y4:32:TYR:OH   | 2.23                     | 0.87              |
| 25:YA:1533:C:N4    | 25:YA:1538:G:H1   | 1.73                     | 0.86              |
| 25:RA:2287:A:H62   | 25:RA:2344:U:H3   | 0.90                     | 0.86              |
| 35:RP:19:VAL:HG13  | 35:RP:21:ARG:H    | 1.40                     | 0.86              |
| 25:YA:1138:G:H21   | 33:YN:106:MET:HE3 | 1.41                     | 0.86              |
| 25:RA:1169:G:N2    | 25:RA:1180:C:N3   | 2.23                     | 0.86              |
| 25:RA:847:U:O4     | 25:RA:933:A:N1    | 2.08                     | 0.86              |
| 1:QA:1316:G:H22    | 1:QA:1319:A:H5''  | 1.41                     | 0.86              |
| 1:XA:1298:C:OP2    | 7:XG:114:ARG:NH2  | 2.07                     | 0.86              |
| 4:XD:9:CYS:SG      | 4:XD:22:LYS:CE    | 2.63                     | 0.86              |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:H   | 1.39                     | 0.86              |
| 51:R5:50:GLY:HA3   | 51:R5:56:LYS:CB   | 2.06                     | 0.86              |
| 1:XA:963:G:H1      | 1:XA:972:C:N4     | 1.73                     | 0.86              |
| 4:XD:157:LEU:O     | 4:XD:161:ASN:ND2  | 2.07                     | 0.86              |
| 27:RD:43:ARG:NH1   | 27:RD:44:ASN:OD1  | 2.09                     | 0.85              |
| 1:QA:410:G:H3'     | 4:QD:25:ARG:HH21  | 1.41                     | 0.85              |
| 5:QE:50:GLU:HB3    | 5:QE:53:LEU:HD13  | 1.59                     | 0.85              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 32:RI:53:ALA:O    | 32:RI:57:ARG:HG3    | 1.77                     | 0.85              |
| 25:RA:806:C:OP2   | 35:RP:41:ARG:NH1    | 2.09                     | 0.85              |
| 42:YW:18:ARG:HG3  | 42:YW:76:VAL:HG13   | 1.58                     | 0.85              |
| 44:RY:79:CYS:SG   | 44:RY:80:GLY:N      | 2.45                     | 0.84              |
| 4:QD:195:ALA:HB3  | 6:XF:16:GLN:O       | 1.76                     | 0.84              |
| 25:RA:1043:C:N3   | 25:RA:1112:G:N2     | 2.25                     | 0.84              |
| 26:RB:33:G:H5'    | 30:RG:2:PRO:HG3     | 1.59                     | 0.84              |
| 19:XS:42:PRO:CB   | 50:Y4:60:GLN:OE1    | 2.26                     | 0.84              |
| 35:YP:58:THR:O    | 35:YP:61:ARG:NE     | 2.09                     | 0.84              |
| 25:RA:49:A:N7     | 25:RA:120:U:C4      | 2.45                     | 0.84              |
| 19:QS:9:VAL:CG1   | 50:R4:66:SER:O      | 2.24                     | 0.84              |
| 19:XS:65:ASN:HA   | 50:Y4:55:ARG:HD2    | 1.60                     | 0.84              |
| 39:YT:26:ASP:HB3  | 39:YT:92:GLY:H      | 1.42                     | 0.84              |
| 32:RI:52:ARG:HB2  | 32:RI:56:LYS:CB     | 2.08                     | 0.84              |
| 1:QA:1002:G:H1    | 1:QA:1038:C:N4      | 1.75                     | 0.84              |
| 19:XS:68:GLY:N    | 50:Y4:59:PHE:CE1    | 2.46                     | 0.84              |
| 25:RA:1043:C:N4   | 25:RA:1112:G:H1     | 1.74                     | 0.84              |
| 33:YN:4:TYR:O     | 40:YU:64:ARG:NH1    | 2.10                     | 0.84              |
| 56:Z7:1:T17:H66   | 56:Z7:2:GLY:H       | 1.41                     | 0.84              |
| 25:YA:67:U:H3     | 25:YA:74:A:H2       | 1.25                     | 0.84              |
| 25:YA:631:A:OP2   | 54:Y8:46:ARG:NH2    | 2.11                     | 0.83              |
| 2:QB:80:ILE:HD11  | 2:QB:208:ILE:HG23   | 1.58                     | 0.83              |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:HG12  | 1.59                     | 0.83              |
| 6:QF:17:SER:O     | 6:QF:20:ALA:N       | 2.11                     | 0.83              |
| 25:YA:2098:U:H3   | 25:YA:2191:G:H1     | 1.26                     | 0.83              |
| 25:RA:1359:A:N1   | 25:RA:1372:U:O4     | 2.11                     | 0.83              |
| 31:YH:12:PRO:HD3  | 31:YH:48:GLY:O      | 1.77                     | 0.83              |
| 25:YA:483:A:H4'   | 44:YY:49:VAL:HA     | 1.59                     | 0.83              |
| 30:YG:27:ASN:HB3  | 30:YG:30:GLU:HG3    | 1.60                     | 0.83              |
| 35:YP:19:VAL:HG13 | 35:YP:21:ARG:H      | 1.41                     | 0.83              |
| 1:XA:963:G:N3     | 10:XJ:55:LYS:NZ     | 2.27                     | 0.83              |
| 25:RA:857:C:H4'   | 46:R0:23:VAL:HG21   | 1.59                     | 0.83              |
| 40:YU:90:VAL:O    | 40:YU:92:ARG:N      | 2.11                     | 0.82              |
| 25:RA:530:G:O2'   | 25:RA:532:A:N7      | 2.12                     | 0.82              |
| 32:RI:55:ALA:O    | 32:RI:58:LEU:HB3    | 1.78                     | 0.82              |
| 19:XS:5:LEU:HG    | 50:Y4:66:SER:CB     | 2.09                     | 0.82              |
| 25:YA:1021:A:H61  | 25:YA:1142(A):A:H61 | 1.22                     | 0.82              |
| 4:QD:195:ALA:CB   | 6:XF:20:ALA:HB2     | 2.09                     | 0.82              |
| 51:R5:4:HIS:HB3   | 51:R5:5:PRO:HD3     | 1.62                     | 0.82              |
| 28:RE:20:ALA:C    | 28:RE:21:VAL:HG13   | 1.97                     | 0.82              |
| 4:XD:9:CYS:SG     | 4:XD:22:LYS:HE2     | 2.19                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:QF:17:SER:O      | 6:QF:19:LEU:N      | 2.12                     | 0.82              |
| 25:YA:620:G:H4'    | 25:YA:621:A:H5''   | 1.60                     | 0.82              |
| 25:YA:2015:A:H1'   | 51:Y5:2:ALA:HA     | 1.60                     | 0.82              |
| 51:R5:16:ARG:NH1   | 51:R5:17:ASP:OD1   | 2.13                     | 0.82              |
| 1:XA:31:G:O2'      | 1:XA:48:C:N4       | 2.11                     | 0.82              |
| 42:YW:90:ARG:HH11  | 42:YW:90:ARG:HG3   | 1.45                     | 0.82              |
| 29:RF:197:ASP:O    | 29:RF:199:TRP:N    | 2.12                     | 0.82              |
| 25:YA:2753:A:O2'   | 55:Y9:15:LYS:NZ    | 2.12                     | 0.82              |
| 44:RY:29:GLU:HB3   | 44:RY:38:ILE:HG12  | 1.62                     | 0.82              |
| 28:RE:22:PRO:HD2   | 28:RE:185:LYS:HD2  | 1.61                     | 0.81              |
| 25:RA:2308:G:N1    | 25:RA:2311:A:C2    | 2.47                     | 0.81              |
| 47:Y1:7:ILE:HD12   | 47:Y1:62:VAL:HG11  | 1.62                     | 0.81              |
| 4:QD:167:GLY:CA    | 27:YD:135:PHE:HE1  | 1.83                     | 0.81              |
| 19:QS:68:GLY:HA3   | 50:R4:68:ARG:HB2   | 1.62                     | 0.81              |
| 25:RA:2068:U:H3    | 25:RA:2430:A:H2    | 1.28                     | 0.81              |
| 28:RE:15:PHE:CD1   | 28:RE:20:ALA:HB2   | 2.14                     | 0.81              |
| 51:Y5:16:ARG:NH1   | 51:Y5:17:ASP:OD1   | 2.13                     | 0.81              |
| 25:YA:265:A:N6     | 25:YA:427:U:O2'    | 2.13                     | 0.81              |
| 25:YA:1664:A:H61   | 25:YA:1996:C:H42   | 1.29                     | 0.81              |
| 35:RP:62:LEU:HD21  | 54:R8:25:MET:HB2   | 1.61                     | 0.81              |
| 33:YN:4:TYR:OH     | 33:YN:7:LYS:NZ     | 2.14                     | 0.81              |
| 29:RF:103:LYS:HA   | 29:RF:106:ARG:HG3  | 1.63                     | 0.81              |
| 1:XA:1002:G:H1     | 1:XA:1038:C:H42    | 1.27                     | 0.81              |
| 48:Y2:47:ASN:O     | 48:Y2:49:LYS:N     | 2.12                     | 0.81              |
| 19:QS:70:LYS:CE    | 50:R4:68:ARG:NH2   | 2.43                     | 0.81              |
| 13:QM:14:ARG:H     | 13:QM:44:ARG:HD3   | 1.45                     | 0.81              |
| 48:R2:47:ASN:O     | 48:R2:49:LYS:N     | 2.13                     | 0.81              |
| 2:XB:69:LEU:HB3    | 2:XB:162:ILE:HG22  | 1.61                     | 0.81              |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:H    | 1.45                     | 0.81              |
| 39:RT:24:PRO:HA    | 39:RT:49:VAL:HG13  | 1.61                     | 0.80              |
| 25:RA:676:A:H8     | 25:RA:2069:G:H21   | 1.29                     | 0.80              |
| 31:YH:10:PRO:CD    | 31:YH:50:VAL:O     | 2.29                     | 0.80              |
| 4:QD:30:LYS:C      | 4:QD:32:ALA:H      | 1.83                     | 0.80              |
| 25:RA:273:G:H1     | 25:RA:364:C:H42    | 1.27                     | 0.80              |
| 45:RZ:108:PRO:HA   | 45:RZ:142:SER:HA   | 1.60                     | 0.80              |
| 25:YA:1824:G:OP1   | 27:YD:52:ARG:NH1   | 2.14                     | 0.80              |
| 32:YI:92:VAL:HG13  | 32:YI:120:ILE:HG23 | 1.64                     | 0.80              |
| 25:YA:956:G:H5''   | 36:YQ:77:LYS:HE2   | 1.64                     | 0.80              |
| 28:RE:50:GLY:HA2   | 28:RE:77:ILE:HA    | 1.64                     | 0.80              |
| 33:RN:42:TRP:O     | 40:RU:64:ARG:NH2   | 2.15                     | 0.80              |
| 32:YI:130:TYR:HB3  | 32:YI:136:VAL:HG13 | 1.62                     | 0.80              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:847:U:C4      | 25:RA:933:A:N1     | 2.50                     | 0.80              |
| 25:RA:958:U:OP2     | 36:RQ:14:ARG:NH1   | 2.13                     | 0.80              |
| 25:RA:270(R):G:N3   | 47:R1:78:LYS:NZ    | 2.30                     | 0.80              |
| 44:YY:76:CYS:SG     | 44:YY:77:PRO:HD2   | 2.22                     | 0.80              |
| 13:QM:3:ARG:HA      | 13:QM:9:ILE:HG21   | 1.62                     | 0.80              |
| 25:RA:768:G:O2'     | 25:RA:1379:A:N6    | 2.14                     | 0.80              |
| 25:YA:1359:A:N6     | 25:YA:1372:U:C4    | 2.50                     | 0.80              |
| 25:RA:2445:G:OP1    | 29:RF:74:ARG:NH2   | 2.15                     | 0.80              |
| 13:XM:65:LYS:HD3    | 13:XM:69:GLU:HG3   | 1.63                     | 0.79              |
| 25:YA:2580:U:H4'    | 28:YE:130:GLY:HA3  | 1.65                     | 0.79              |
| 56:Z8:1:T17:H66     | 56:Z8:2:GLY:H      | 1.46                     | 0.79              |
| 1:XA:1108:G:H5'     | 3:XC:176:HIS:HD1   | 1.47                     | 0.79              |
| 3:XC:32:LEU:HD13    | 3:XC:59:ARG:HD3    | 1.64                     | 0.79              |
| 25:YA:1169:G:N2     | 25:YA:1180:C:N3    | 2.30                     | 0.79              |
| 43:YX:67:GLY:O      | 43:YX:69:TYR:N     | 2.15                     | 0.79              |
| 31:YH:10:PRO:CD     | 31:YH:50:VAL:HG13  | 2.13                     | 0.79              |
| 45:YZ:182:LYS:HG3   | 45:YZ:183:LEU:HD23 | 1.62                     | 0.79              |
| 37:RR:104:ARG:HD2   | 37:RR:111:LEU:HD21 | 1.63                     | 0.79              |
| 1:QA:346:G:OP1      | 39:RT:41:ARG:NH2   | 2.15                     | 0.79              |
| 11:QK:21:ILE:HB     | 11:QK:84:VAL:HG12  | 1.65                     | 0.79              |
| 2:XB:77:ALA:HB2     | 2:XB:211:ILE:HD13  | 1.64                     | 0.79              |
| 25:YA:780:G:H21     | 25:YA:783:A:H62    | 1.30                     | 0.79              |
| 1:QA:1392:G:H21     | 1:QA:1502:A:H8     | 1.29                     | 0.79              |
| 15:QO:26:GLU:OE2    | 15:QO:77:ARG:NH1   | 2.16                     | 0.79              |
| 20:XT:33:ILE:O      | 20:XT:37:SER:OG    | 2.00                     | 0.79              |
| 35:YP:62:LEU:H      | 35:YP:62:LEU:HD23  | 1.46                     | 0.79              |
| 6:QF:15:ASP:OD1     | 6:QF:17:SER:HB2    | 1.83                     | 0.79              |
| 19:QS:67:VAL:HG12   | 50:R4:59:PHE:CD1   | 2.15                     | 0.79              |
| 25:RA:978:G:H1      | 25:RA:985:C:H42    | 1.28                     | 0.79              |
| 45:YZ:144:LEU:HD11  | 45:YZ:149:SER:HA   | 1.63                     | 0.79              |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:HD22  | 1.65                     | 0.78              |
| 1:XA:664:G:H22      | 1:XA:741:G:H1      | 1.31                     | 0.78              |
| 8:QH:91:ARG:HB2     | 12:QL:7:ILE:HG13   | 1.65                     | 0.78              |
| 25:RA:1048:A:H2     | 25:RA:1112:G:H21   | 1.32                     | 0.78              |
| 45:RZ:108:PRO:HG2   | 45:RZ:110:GLY:O    | 1.84                     | 0.78              |
| 3:XC:59:ARG:HH12    | 3:XC:97:LYS:HE3    | 1.48                     | 0.78              |
| 6:XF:50:TYR:OH      | 18:XR:74:ARG:O     | 2.00                     | 0.78              |
| 13:QM:8:GLU:OE2     | 30:RG:115:ARG:HD3  | 1.84                     | 0.78              |
| 35:RP:126:VAL:HG12  | 35:RP:147:LEU:HD21 | 1.63                     | 0.78              |
| 4:XD:9:CYS:SG       | 4:XD:22:LYS:NZ     | 2.52                     | 0.78              |
| 33:RN:95:PRO:O      | 33:RN:97:ARG:N     | 2.15                     | 0.78              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 19:XS:5:LEU:CG     | 50:Y4:66:SER:HB2    | 2.14                     | 0.78              |
| 51:R5:56:LYS:HE2   | 51:R5:58:LEU:CD2    | 2.14                     | 0.78              |
| 12:XL:50:SER:O     | 12:XL:51:ALA:HB2    | 1.82                     | 0.78              |
| 50:Y4:1:MET:SD     | 50:Y4:6:HIS:NE2     | 2.56                     | 0.78              |
| 27:YD:121:PRO:HB3  | 27:YD:135:PHE:CZ    | 2.19                     | 0.78              |
| 20:QT:100:ILE:HG13 | 20:QT:102:GLY:H     | 1.48                     | 0.78              |
| 25:YA:847:U:C4     | 25:YA:933:A:N1      | 2.51                     | 0.78              |
| 10:QJ:50:ILE:HA    | 10:QJ:60:ARG:HG2    | 1.66                     | 0.78              |
| 27:RD:69:ARG:NH2   | 27:RD:128:GLY:O     | 2.17                     | 0.78              |
| 4:QD:167:GLY:HA2   | 27:YD:135:PHE:CE1   | 2.16                     | 0.78              |
| 27:YD:248:SER:CB   | 27:YD:252:TRP:CE2   | 2.66                     | 0.78              |
| 31:YH:10:PRO:HG2   | 31:YH:50:VAL:CG1    | 2.13                     | 0.78              |
| 25:RA:1359:A:C6    | 25:RA:1372:U:O4     | 2.37                     | 0.78              |
| 13:XM:14:ARG:H     | 13:XM:44:ARG:HD3    | 1.49                     | 0.78              |
| 32:RI:4:ILE:HD11   | 32:RI:44:LEU:HD12   | 1.66                     | 0.77              |
| 19:XS:5:LEU:HG     | 50:Y4:66:SER:HB3    | 1.66                     | 0.77              |
| 25:RA:2308:G:N1    | 25:RA:2311:A:H2     | 1.82                     | 0.77              |
| 3:XC:20:SER:HB2    | 3:XC:40:ARG:HH22    | 1.50                     | 0.77              |
| 34:YO:88:ASN:HD21  | 34:YO:92:GLU:HB2    | 1.47                     | 0.77              |
| 25:RA:1311:G:N2    | 25:RA:1603:A:H62    | 1.83                     | 0.77              |
| 25:RA:590:A:OP1    | 29:RF:95:ARG:NH1    | 2.17                     | 0.77              |
| 1:XA:1298:C:H2'    | 7:XG:114:ARG:HH12   | 1.47                     | 0.77              |
| 56:Z7:1:T17:H10    | 56:Z7:1:T17:H55     | 1.65                     | 0.77              |
| 27:YD:69:ARG:NH2   | 27:YD:128:GLY:O     | 2.17                     | 0.77              |
| 51:Y5:38:ALA:HB3   | 51:Y5:40:LYS:HE3    | 1.67                     | 0.77              |
| 25:RA:2807:G:N1    | 25:RA:2893:G:O6     | 2.17                     | 0.77              |
| 29:RF:66:PRO:O     | 29:RF:68:LYS:N      | 2.18                     | 0.77              |
| 33:YN:95:PRO:O     | 33:YN:97:ARG:N      | 2.18                     | 0.77              |
| 25:RA:1021:A:H61   | 25:RA:1142(A):A:H61 | 1.29                     | 0.77              |
| 39:RT:41:ARG:NH1   | 39:RT:41:ARG:HB2    | 1.99                     | 0.77              |
| 1:QA:1502:A:H2     | 1:QA:1505:G:H1      | 1.33                     | 0.77              |
| 51:R5:35:GLU:HB3   | 51:R5:49:CYS:SG     | 2.25                     | 0.77              |
| 1:XA:261:U:OP2     | 20:XT:79:ARG:NH2    | 2.17                     | 0.77              |
| 25:YA:2068:U:H3    | 25:YA:2430:A:H2     | 1.32                     | 0.77              |
| 35:YP:47:ASP:OD2   | 35:YP:50:ARG:NH2    | 2.17                     | 0.77              |
| 1:QA:1243:C:OP2    | 21:QU:10:ARG:NH2    | 2.18                     | 0.77              |
| 25:RA:873:G:H1     | 25:RA:904:C:H42     | 1.31                     | 0.77              |
| 31:RH:125:VAL:CG1  | 31:RH:126:PRO:CG    | 2.63                     | 0.77              |
| 1:XA:1368:G:OP1    | 9:XI:111:ARG:NH2    | 2.17                     | 0.76              |
| 42:YW:90:ARG:HG3   | 42:YW:90:ARG:NH1    | 2.00                     | 0.76              |
| 25:YA:2287:A:N6    | 25:YA:2344:U:H3     | 1.82                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:QM:80:ARG:CD   | 50:R4:71:ARG:HH22 | 1.99                     | 0.76              |
| 25:YA:242:G:H5'   | 54:Y8:62:LEU:HD13 | 1.67                     | 0.76              |
| 25:YA:49:A:N7     | 25:YA:120:U:O4    | 2.18                     | 0.76              |
| 19:QS:67:VAL:CG1  | 50:R4:59:PHE:CE1  | 2.68                     | 0.76              |
| 28:RE:9:VAL:HB    | 28:RE:25:VAL:HG23 | 1.66                     | 0.76              |
| 37:RR:3:HIS:O     | 37:RR:5:LYS:N     | 2.19                     | 0.76              |
| 23:QW:12:U:H3     | 23:QW:23:A:H61    | 1.33                     | 0.76              |
| 26:RB:40:U:O2     | 26:RB:45:A:N6     | 2.19                     | 0.76              |
| 1:XA:1305:G:H22   | 1:XA:1331:G:H2'   | 1.51                     | 0.76              |
| 1:QA:31:G:O2'     | 1:QA:48:C:N4      | 2.18                     | 0.76              |
| 43:RX:60:ARG:NH1  | 53:R7:47:ARG:HH22 | 1.83                     | 0.76              |
| 1:XA:880:C:OP1    | 12:XL:12:ARG:NH1  | 2.18                     | 0.76              |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:H    | 1.51                     | 0.76              |
| 13:QM:80:ARG:NE   | 50:R4:71:ARG:HH12 | 1.83                     | 0.76              |
| 19:XS:9:VAL:HG13  | 50:Y4:66:SER:O    | 1.86                     | 0.76              |
| 29:YF:197:ASP:O   | 29:YF:199:TRP:N   | 2.19                     | 0.76              |
| 37:YR:74:LYS:O    | 37:YR:76:VAL:N    | 2.18                     | 0.76              |
| 38:RS:62:LYS:HB3  | 38:RS:97:ARG:HD3  | 1.67                     | 0.76              |
| 1:XA:1130:A:O2'   | 9:XI:3:GLN:NE2    | 2.17                     | 0.76              |
| 28:RE:15:PHE:CE1  | 28:RE:20:ALA:HB2  | 2.21                     | 0.75              |
| 25:YA:1169:G:H1   | 25:YA:1180:C:H42  | 0.77                     | 0.75              |
| 25:YA:1607:C:N4   | 25:YA:1622:G:OP2  | 2.19                     | 0.75              |
| 1:QA:1055:A:N7    | 1:QA:1200:C:N4    | 2.34                     | 0.75              |
| 25:YA:1309:G:H4'  | 53:Y7:7:PRO:HB2   | 1.68                     | 0.75              |
| 44:RY:95:LYS:HB3  | 44:RY:100:ALA:HA  | 1.68                     | 0.75              |
| 19:XS:5:LEU:HD11  | 50:Y4:67:TYR:N    | 2.00                     | 0.75              |
| 19:QS:67:VAL:CB   | 50:R4:59:PHE:CZ   | 2.68                     | 0.75              |
| 51:R5:55:ARG:HH11 | 51:R5:57:VAL:HA   | 1.49                     | 0.75              |
| 1:XA:439:A:OP2    | 1:XA:493:G:N1     | 2.19                     | 0.75              |
| 25:YA:2051:A:C2   | 25:YA:2052:G:O6   | 2.40                     | 0.75              |
| 45:YZ:54:HIS:O    | 45:YZ:98:MET:CE   | 2.35                     | 0.75              |
| 25:RA:1071:G:O6   | 25:RA:1091:G:O6   | 2.03                     | 0.75              |
| 44:RY:87:LYS:HD3  | 44:RY:92:ASN:HB3  | 1.69                     | 0.75              |
| 5:QE:102:ALA:HB1  | 5:QE:106:PRO:HG2  | 1.69                     | 0.75              |
| 37:RR:74:LYS:O    | 37:RR:76:VAL:N    | 2.18                     | 0.75              |
| 25:YA:67:U:N3     | 25:YA:74:A:C2     | 2.53                     | 0.75              |
| 39:YT:57:PHE:O    | 39:YT:58:ASN:ND2  | 2.20                     | 0.75              |
| 39:YT:27:THR:HG23 | 39:YT:90:GLN:HB3  | 1.67                     | 0.75              |
| 40:YU:92:ARG:O    | 40:YU:94:ASN:N    | 2.20                     | 0.75              |
| 1:XA:1128:C:N3    | 1:XA:1144:G:N2    | 2.35                     | 0.75              |
| 52:R6:41:PRO:HG2  | 52:R6:45:LYS:H    | 1.52                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RP:14:LYS:O     | 35:RP:16:ARG:N     | 2.20                     | 0.75              |
| 44:RY:86:ARG:HB2   | 44:RY:95:LYS:HD2   | 1.69                     | 0.75              |
| 1:XA:971:G:N2      | 1:XA:1363:A:OP2    | 2.20                     | 0.75              |
| 19:XS:3:ARG:HB3    | 50:Y4:67:TYR:CD2   | 2.22                     | 0.75              |
| 25:YA:888:C:H3'    | 25:YA:889:C:H4'    | 1.69                     | 0.75              |
| 51:R5:58:LEU:N     | 51:R5:58:LEU:HD12  | 2.02                     | 0.74              |
| 25:RA:155:C:H42    | 25:RA:171:G:H1     | 1.35                     | 0.74              |
| 33:YN:13:TRP:HB2   | 33:YN:133:GLN:HG3  | 1.69                     | 0.74              |
| 1:QA:345:C:OP1     | 39:RT:41:ARG:NH1   | 2.20                     | 0.74              |
| 37:RR:56:LYS:NZ    | 37:RR:90:ARG:O     | 2.20                     | 0.74              |
| 1:XA:1129:C:N4     | 1:XA:1133:G:O6     | 2.19                     | 0.74              |
| 17:XQ:66:SER:O     | 17:XQ:70:ARG:NH1   | 2.20                     | 0.74              |
| 41:YV:24:LYS:HA    | 41:YV:92:THR:HG23  | 1.68                     | 0.74              |
| 8:QH:29:SER:HB3    | 8:QH:32:LYS:HG3    | 1.69                     | 0.74              |
| 25:RA:674:G:H1'    | 29:RF:74:ARG:HD3   | 1.69                     | 0.74              |
| 30:RG:34:LEU:HB2   | 30:RG:172:LEU:HD21 | 1.68                     | 0.74              |
| 13:XM:3:ARG:HH22   | 30:YG:139:LEU:HD13 | 1.50                     | 0.74              |
| 45:RZ:60:GLU:HA    | 45:RZ:66:SER:HA    | 1.68                     | 0.74              |
| 38:YS:78:LEU:HD21  | 38:YS:108:GLY:HA3  | 1.68                     | 0.74              |
| 5:QE:7:GLU:HG2     | 5:QE:112:LEU:HD22  | 1.69                     | 0.74              |
| 11:XK:54:ARG:NH2   | 23:XW:39:U:O3'     | 2.20                     | 0.74              |
| 39:YT:51:ARG:HG2   | 39:YT:98:LYS:HG3   | 1.70                     | 0.74              |
| 45:YZ:30:ASN:HD22  | 45:YZ:90:VAL:HB    | 1.51                     | 0.74              |
| 25:RA:631:A:OP2    | 54:R8:46:ARG:NH2   | 2.19                     | 0.74              |
| 1:XA:1422:G:H5''   | 34:YO:48:PRO:HB3   | 1.69                     | 0.74              |
| 28:YE:24:THR:CG2   | 28:YE:188:VAL:HG11 | 2.16                     | 0.74              |
| 29:RF:6:VAL:HB     | 29:RF:24:LEU:CB    | 2.18                     | 0.74              |
| 14:QN:24:CYS:CB    | 14:QN:27:CYS:SG    | 2.74                     | 0.74              |
| 13:XM:62:ASN:HA    | 50:Y4:49:PHE:CD2   | 2.23                     | 0.74              |
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H    | 1.53                     | 0.74              |
| 5:QE:100:VAL:O     | 5:QE:107:ARG:NH2   | 2.20                     | 0.74              |
| 1:QA:658:G:OP1     | 15:QO:8:LYS:NZ     | 2.20                     | 0.74              |
| 28:RE:62:PRO:O     | 28:RE:64:LYS:N     | 2.20                     | 0.74              |
| 31:YH:15:VAL:HG21  | 31:YH:76:VAL:HG13  | 1.68                     | 0.74              |
| 38:YS:56:LEU:HB3   | 38:YS:58:LEU:HD22  | 1.69                     | 0.74              |
| 19:QS:67:VAL:CG1   | 50:R4:59:PHE:CD1   | 2.71                     | 0.74              |
| 45:YZ:95:PRO:CG    | 45:YZ:127:LYS:HD3  | 2.18                     | 0.74              |
| 19:XS:68:GLY:HA3   | 50:Y4:59:PHE:HE1   | 1.52                     | 0.73              |
| 19:XS:5:LEU:HD11   | 50:Y4:66:SER:CA    | 2.18                     | 0.73              |
| 25:YA:630:G:OP1    | 54:Y8:46:ARG:NH1   | 2.21                     | 0.73              |
| 1:QA:963:G:N3      | 10:QJ:55:LYS:NZ    | 2.32                     | 0.73              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:QD:175:SER:HB3   | 4:QD:186:LEU:HD21   | 1.69                     | 0.73              |
| 1:QA:686:U:H1'     | 11:QK:42:TRP:HE1    | 1.51                     | 0.73              |
| 47:R1:7:ILE:HG12   | 47:R1:91:LYS:HZ1    | 1.51                     | 0.73              |
| 53:R7:9:ARG:NH2    | 53:R7:48:LYS:HB2    | 2.03                     | 0.73              |
| 25:RA:1693:U:O2'   | 27:RD:14:ARG:NH2    | 2.21                     | 0.73              |
| 19:XS:68:GLY:CA    | 50:Y4:59:PHE:HE1    | 2.01                     | 0.73              |
| 43:YX:27:THR:HB    | 43:YX:80:ILE:HB     | 1.69                     | 0.73              |
| 1:QA:1086:U:H3     | 1:QA:1099:G:H22     | 1.35                     | 0.73              |
| 50:Y4:9:LEU:H      | 50:Y4:27:THR:HG23   | 1.53                     | 0.73              |
| 1:QA:677:U:H3      | 1:QA:713:G:H22      | 1.36                     | 0.73              |
| 19:QS:70:LYS:NZ    | 50:R4:68:ARG:NH2    | 2.37                     | 0.73              |
| 25:YA:2030:A:H4'   | 25:YA:2031:A:H8     | 1.52                     | 0.73              |
| 35:YP:14:LYS:O     | 35:YP:16:ARG:N      | 2.22                     | 0.73              |
| 13:XM:3:ARG:HG2    | 50:Y4:34:GLU:HG2    | 1.70                     | 0.73              |
| 25:YA:676:A:H8     | 25:YA:2069:G:H21    | 1.33                     | 0.73              |
| 25:YA:483:A:H5'    | 44:YY:49:VAL:HG22   | 1.69                     | 0.73              |
| 45:YZ:158:PRO:O    | 45:YZ:160:GLY:N     | 2.22                     | 0.73              |
| 3:QC:58:GLU:HB2    | 3:QC:65:ALA:HB3     | 1.70                     | 0.73              |
| 4:XD:7:PRO:HB2     | 4:XD:10:ARG:HD2     | 1.69                     | 0.73              |
| 13:XM:11:ARG:HH21  | 30:YG:146:TYR:HD2   | 1.35                     | 0.73              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:H     | 1.53                     | 0.73              |
| 4:QD:30:LYS:N      | 4:QD:30:LYS:HD3     | 2.03                     | 0.73              |
| 36:YQ:24:GLY:O     | 36:YQ:26:TYR:N      | 2.19                     | 0.73              |
| 56:Z7:1:T17:H62    | 56:Z7:3:GLY:H       | 1.54                     | 0.73              |
| 53:R7:9:ARG:NH2    | 53:R7:48:LYS:HD2    | 1.98                     | 0.73              |
| 25:RA:1443:G:H1    | 25:RA:1548:C:H42    | 1.35                     | 0.73              |
| 36:YQ:111:GLU:OE1  | 36:YQ:133:ARG:NH2   | 2.22                     | 0.73              |
| 25:RA:1071:G:N1    | 25:RA:1091:G:N7     | 2.33                     | 0.73              |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:N     | 2.03                     | 0.73              |
| 36:YQ:104:PHE:HE2  | 36:YQ:125:LEU:HD11  | 1.54                     | 0.73              |
| 1:QA:261:U:OP2     | 20:QT:79:ARG:NH2    | 2.22                     | 0.72              |
| 13:QM:80:ARG:HD3   | 50:R4:71:ARG:CZ     | 2.19                     | 0.72              |
| 25:RA:1019:U:H3    | 25:RA:1142(A):A:H62 | 1.37                     | 0.72              |
| 25:RA:1310:G:OP2   | 53:R7:9:ARG:NH1     | 2.22                     | 0.72              |
| 25:RA:1607:C:N4    | 25:RA:1622:G:OP2    | 2.22                     | 0.72              |
| 25:RA:392:C:H5''   | 25:RA:409:C:H5''    | 1.70                     | 0.72              |
| 1:XA:973:G:OP1     | 10:XJ:57:LYS:NZ     | 2.22                     | 0.72              |
| 25:YA:1509:C:H3'   | 25:YA:1510:A:H5''   | 1.71                     | 0.72              |
| 25:YA:587:C:OP2    | 35:YP:21:ARG:NH2    | 2.21                     | 0.72              |
| 7:QG:9:VAL:HG13    | 7:QG:94:ARG:HH21    | 1.54                     | 0.72              |
| 25:RA:1411:C:H42   | 25:RA:1591:G:H1     | 1.34                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:882:G:H1     | 25:RA:894:C:H42    | 1.35                     | 0.72              |
| 32:RI:5:LEU:HD11   | 32:RI:19:VAL:HG12  | 1.70                     | 0.72              |
| 50:Y4:48:ARG:HH12  | 50:Y4:52:THR:HG22  | 1.54                     | 0.72              |
| 25:YA:2701:C:H3'   | 25:YA:2702:U:C5'   | 2.19                     | 0.72              |
| 3:QC:20:SER:HB2    | 3:QC:40:ARG:HH22   | 1.54                     | 0.72              |
| 25:RA:2502:G:H5''  | 25:RA:2503:A:H5''  | 1.70                     | 0.72              |
| 1:XA:1086:U:H3     | 1:XA:1099:G:H22    | 1.36                     | 0.72              |
| 32:YI:144:VAL:HG13 | 32:YI:145:VAL:HG13 | 1.70                     | 0.72              |
| 28:RE:21:VAL:HG23  | 28:RE:22:PRO:N     | 2.05                     | 0.72              |
| 30:YG:64:THR:HG23  | 30:YG:66:GLN:H     | 1.55                     | 0.72              |
| 25:RA:884:C:O2     | 25:RA:892:G:N1     | 2.23                     | 0.72              |
| 44:YY:51:VAL:HG13  | 44:YY:52:SER:H     | 1.54                     | 0.72              |
| 17:QQ:4:LYS:HE3    | 17:QQ:6:LEU:HD21   | 1.72                     | 0.72              |
| 31:RH:125:VAL:CG1  | 31:RH:126:PRO:HG3  | 2.20                     | 0.72              |
| 32:RI:93:THR:HG22  | 32:RI:119:PRO:HB3  | 1.72                     | 0.72              |
| 30:YG:6:ALA:H      | 50:Y4:23:GLU:HG2   | 1.54                     | 0.72              |
| 25:YA:1190:G:OP1   | 35:YP:30:THR:OG1   | 2.06                     | 0.72              |
| 1:XA:243:A:H4'     | 1:XA:244:U:H3'     | 1.70                     | 0.72              |
| 27:YD:35:LYS:HD2   | 27:YD:104:TYR:CE1  | 2.25                     | 0.72              |
| 45:YZ:91:LEU:CD1   | 45:YZ:96:VAL:HG21  | 2.20                     | 0.72              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:HG3  | 1.70                     | 0.72              |
| 19:XS:5:LEU:HD11   | 50:Y4:66:SER:HB2   | 1.71                     | 0.72              |
| 48:Y2:42:GLY:O     | 48:Y2:44:LEU:N     | 2.20                     | 0.72              |
| 31:YH:129:THR:OG1  | 31:YH:129:THR:O    | 2.08                     | 0.72              |
| 34:YO:47:ILE:HG13  | 34:YO:48:PRO:HD2   | 1.72                     | 0.72              |
| 45:YZ:96:VAL:HG12  | 45:YZ:128:VAL:O    | 1.89                     | 0.72              |
| 46:R0:68:GLU:OE1   | 46:R0:82:ARG:NH1   | 2.23                     | 0.71              |
| 1:XA:564:C:O2'     | 8:XH:91:ARG:NH2    | 2.23                     | 0.71              |
| 12:QL:7:ILE:HG21   | 17:QQ:34:LYS:HB2   | 1.71                     | 0.71              |
| 45:YZ:103:ARG:HB2  | 45:YZ:138:GLU:HG2  | 1.72                     | 0.71              |
| 51:R5:56:LYS:O     | 51:R5:57:VAL:HG12  | 1.89                     | 0.71              |
| 25:RA:987:G:O2'    | 25:RA:1000:A:N3    | 2.20                     | 0.71              |
| 25:RA:1138:G:H21   | 33:RN:106:MET:HE3  | 1.54                     | 0.71              |
| 36:RQ:81:VAL:C     | 36:RQ:82:ARG:HG2   | 2.10                     | 0.71              |
| 45:RZ:166:SER:HB2  | 45:RZ:168:GLU:N    | 2.05                     | 0.71              |
| 9:XI:114:TYR:HE2   | 10:XJ:60:ARG:H     | 1.38                     | 0.71              |
| 31:YH:153:LYS:HG2  | 31:YH:162:ILE:HG13 | 1.72                     | 0.71              |
| 19:QS:67:VAL:N     | 50:R4:59:PHE:CZ    | 2.59                     | 0.71              |
| 4:QD:159:ARG:NH2   | 25:YA:2197:U:OP1   | 2.22                     | 0.71              |
| 28:YE:170:LEU:HD21 | 28:YE:187:ALA:HB3  | 1.72                     | 0.71              |
| 52:R6:17:LYS:HB3   | 52:R6:44:ARG:HH22  | 1.55                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:24:LEU:HG    | 29:RF:115:ALA:HB2  | 1.72                     | 0.71              |
| 5:XE:10:MET:HB3    | 5:XE:32:VAL:HG22   | 1.70                     | 0.71              |
| 38:YS:24:LEU:HB2   | 38:YS:85:VAL:HG12  | 1.70                     | 0.71              |
| 45:YZ:102:LEU:HG   | 45:YZ:123:ASP:HA   | 1.72                     | 0.71              |
| 10:QJ:61:GLU:OE2   | 14:QN:45:ARG:NH1   | 2.23                     | 0.71              |
| 49:R3:8:LEU:HD13   | 49:R3:31:LEU:HD23  | 1.71                     | 0.71              |
| 35:RP:38:GLN:HG2   | 35:RP:45:LEU:HD12  | 1.72                     | 0.71              |
| 25:YA:2315:G:OP1   | 30:YG:36:LYS:NZ    | 2.24                     | 0.71              |
| 51:R5:52:TYR:O     | 51:R5:53:ALA:CB    | 2.37                     | 0.71              |
| 8:XH:10:LEU:HD22   | 8:XH:83:ILE:HD11   | 1.72                     | 0.71              |
| 33:YN:89:LYS:O     | 33:YN:93:THR:HG22  | 1.90                     | 0.71              |
| 39:YT:77:PRO:HB2   | 39:YT:80:SER:HB2   | 1.72                     | 0.71              |
| 2:QB:115:LEU:HB2   | 2:QB:145:LEU:HD12  | 1.73                     | 0.71              |
| 30:RG:61:ALA:HB2   | 30:RG:68:PRO:HD3   | 1.72                     | 0.71              |
| 20:XT:45:GLN:HB2   | 20:XT:91:LEU:HD13  | 1.73                     | 0.71              |
| 25:YA:1310:G:OP2   | 53:Y7:9:ARG:NH1    | 2.24                     | 0.71              |
| 38:YS:106:ARG:HA   | 38:YS:110:LEU:HD21 | 1.73                     | 0.71              |
| 44:YY:42:VAL:HG12  | 44:YY:65:ALA:HB3   | 1.71                     | 0.71              |
| 25:RA:1045:A:C8    | 25:RA:1111:A:N6    | 2.59                     | 0.71              |
| 1:XA:953:G:H5'     | 1:XA:965:A:H61     | 1.55                     | 0.71              |
| 34:YO:2:ILE:HD12   | 34:YO:6:THR:HG21   | 1.72                     | 0.71              |
| 23:XW:8:U:O2'      | 23:XW:21:A:N1      | 2.23                     | 0.70              |
| 44:YY:29:GLU:HB3   | 44:YY:38:ILE:HG23  | 1.70                     | 0.70              |
| 48:R2:29:LYS:HE3   | 48:R2:57:ILE:HG21  | 1.73                     | 0.70              |
| 54:Y8:58:ILE:HD13  | 54:Y8:61:LEU:HD21  | 1.73                     | 0.70              |
| 1:QA:1204:A:OP1    | 14:QN:3:ARG:NH2    | 2.24                     | 0.70              |
| 31:RH:106:THR:HG22 | 31:RH:112:PRO:HB3  | 1.72                     | 0.70              |
| 32:RI:98:ALA:HB2   | 32:RI:111:PRO:HB3  | 1.72                     | 0.70              |
| 1:XA:954:G:H21     | 1:XA:1227:A:N6     | 1.84                     | 0.70              |
| 4:QD:195:ALA:HB2   | 6:XF:20:ALA:HB2    | 1.73                     | 0.70              |
| 10:XJ:50:ILE:HA    | 10:XJ:60:ARG:HG2   | 1.72                     | 0.70              |
| 25:YA:2287:A:N6    | 25:YA:2344:U:N3    | 2.37                     | 0.70              |
| 27:YD:43:ARG:HB3   | 27:YD:54:ARG:HB2   | 1.74                     | 0.70              |
| 30:YG:47:LYS:HD3   | 30:YG:81:LYS:HB2   | 1.73                     | 0.70              |
| 13:QM:59:TYR:O     | 13:QM:63:THR:OG1   | 2.07                     | 0.70              |
| 25:RA:1543:A:H1'   | 25:RA:1545:A:C4'   | 2.21                     | 0.70              |
| 42:RW:29:LEU:HD22  | 42:RW:69:LEU:HD11  | 1.72                     | 0.70              |
| 25:YA:602:G:HO2'   | 25:YA:604:G:HO2'   | 1.34                     | 0.70              |
| 35:YP:62:LEU:N     | 35:YP:62:LEU:HD23  | 2.05                     | 0.70              |
| 42:YW:17:VAL:HG12  | 42:YW:76:VAL:HG11  | 1.72                     | 0.70              |
| 3:QC:79:ARG:HH21   | 11:XK:96:ARG:HG3   | 1.55                     | 0.70              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:QM:7:VAL:CG2     | 30:RG:113:ARG:O    | 2.37                     | 0.70              |
| 19:QS:40:ILE:HD11   | 19:QS:62:ILE:HD12  | 1.74                     | 0.70              |
| 19:QS:41:VAL:HB     | 19:QS:42:PRO:HA    | 1.74                     | 0.70              |
| 10:XJ:61:GLU:OE2    | 14:XN:45:ARG:NH1   | 2.25                     | 0.70              |
| 18:XR:58:LEU:HD23   | 18:XR:62:GLU:HB3   | 1.74                     | 0.70              |
| 19:XS:5:LEU:HD12    | 50:Y4:66:SER:HA    | 1.73                     | 0.70              |
| 13:XM:80:ARG:HE     | 50:Y4:71:ARG:HH22  | 1.39                     | 0.70              |
| 25:RA:1061:U:H5'    | 25:RA:1070:A:H1'   | 1.74                     | 0.70              |
| 19:XS:5:LEU:CD1     | 50:Y4:66:SER:HA    | 2.22                     | 0.70              |
| 45:YZ:54:HIS:O      | 45:YZ:98:MET:HE1   | 1.91                     | 0.70              |
| 25:YA:1667:G:O2'    | 25:YA:1991:U:O4    | 2.09                     | 0.70              |
| 29:YF:185:ASP:HA    | 29:YF:188:ARG:HD3  | 1.72                     | 0.70              |
| 39:RT:18:ASP:N      | 39:RT:18:ASP:OD1   | 2.20                     | 0.70              |
| 1:QA:259:G:H1       | 1:QA:267:C:H42     | 1.38                     | 0.70              |
| 1:QA:589:C:H42      | 1:QA:650:G:H1      | 1.40                     | 0.70              |
| 25:RA:1543:A:O2'    | 25:RA:1544:C:H3'   | 1.90                     | 0.70              |
| 32:RI:52:ARG:O      | 32:RI:56:LYS:CB    | 2.39                     | 0.70              |
| 1:XA:1200:C:O2'     | 1:XA:1201:A:OP2    | 2.10                     | 0.70              |
| 13:XM:7:VAL:HG13    | 13:XM:8:GLU:OE2    | 1.92                     | 0.70              |
| 14:XN:48:ALA:HB2    | 14:XN:53:LEU:HD12  | 1.74                     | 0.70              |
| 25:YA:2245:U:H5'    | 25:YA:2246:G:H5'   | 1.73                     | 0.70              |
| 25:YA:250:G:OP2     | 54:Y8:13:ARG:NH2   | 2.25                     | 0.70              |
| 25:YA:498:G:N3      | 44:YY:47:LYS:NZ    | 2.37                     | 0.70              |
| 1:QA:953:G:H5'      | 1:QA:965:A:H61     | 1.55                     | 0.70              |
| 31:RH:125:VAL:CG1   | 31:RH:126:PRO:CD   | 2.48                     | 0.70              |
| 2:XB:185:ILE:HG22   | 2:XB:199:TYR:HB2   | 1.74                     | 0.70              |
| 10:QJ:48:THR:HA     | 10:QJ:62:HIS:HB3   | 1.72                     | 0.69              |
| 25:RA:2404:C:O3'    | 35:RP:77:ARG:NH2   | 2.24                     | 0.69              |
| 25:RA:265:A:N6      | 25:RA:427:U:O2'    | 2.25                     | 0.69              |
| 28:RE:119:ARG:HB3   | 28:RE:120:TRP:CD1  | 2.27                     | 0.69              |
| 19:XS:5:LEU:CD1     | 50:Y4:66:SER:CA    | 2.70                     | 0.69              |
| 1:QA:1263:C:H42     | 1:QA:1272:G:H1     | 1.40                     | 0.69              |
| 50:R4:18:CYS:SG     | 50:R4:19:GLY:N     | 2.65                     | 0.69              |
| 27:RD:93:ALA:HB3    | 27:RD:105:ILE:HG22 | 1.74                     | 0.69              |
| 4:XD:105:VAL:HG13   | 4:XD:110:PHE:HB2   | 1.74                     | 0.69              |
| 45:YZ:80:ARG:HH21   | 45:YZ:82:ARG:HH22  | 1.40                     | 0.69              |
| 25:YA:270(T):G:H5'' | 47:Y1:97:LEU:HD22  | 1.73                     | 0.69              |
| 25:YA:1045:A:C6     | 25:YA:1111:A:N7    | 2.59                     | 0.69              |
| 25:YA:1899:G:H21    | 25:YA:1902:C:N4    | 1.89                     | 0.69              |
| 26:RB:38:C:N4       | 26:RB:44:G:H1      | 1.90                     | 0.69              |
| 1:XA:1008:C:N4      | 1:XA:1021:G:H1     | 1.87                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:182:ASN:ND2  | 29:YF:185:ASP:OD2  | 2.19                     | 0.69              |
| 1:XA:1054:C:OP2    | 1:XA:1197:G:OP2    | 2.10                     | 0.69              |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:H    | 1.56                     | 0.69              |
| 25:YA:372:G:N2     | 25:YA:401:A:OP2    | 2.22                     | 0.69              |
| 25:YA:482:A:H4'    | 44:YY:47:LYS:HD2   | 1.73                     | 0.69              |
| 27:YD:182:LEU:H    | 27:YD:272:ALA:HB3  | 1.56                     | 0.69              |
| 45:YZ:95:PRO:HB2   | 45:YZ:127:LYS:HG2  | 1.73                     | 0.69              |
| 13:XM:53:VAL:HG12  | 13:XM:57:ARG:HH12  | 1.57                     | 0.69              |
| 19:XS:10:PHE:HB2   | 19:XS:39:THR:H     | 1.54                     | 0.69              |
| 50:Y4:56:VAL:HA    | 50:Y4:60:GLN:HB2   | 1.73                     | 0.69              |
| 7:QG:153:HIS:CE1   | 11:QK:57:THR:HG23  | 2.28                     | 0.69              |
| 19:XS:5:LEU:CG     | 50:Y4:66:SER:CB    | 2.70                     | 0.69              |
| 51:Y5:46:CYS:SG    | 51:Y5:50:GLY:HA2   | 2.33                     | 0.69              |
| 52:Y6:11:LEU:HD11  | 52:Y6:51:GLU:HG3   | 1.75                     | 0.69              |
| 27:YD:71:ASP:HB2   | 27:YD:103:ARG:HH22 | 1.58                     | 0.69              |
| 50:R4:7:PRO:HB2    | 50:R4:27:THR:HG21  | 1.74                     | 0.69              |
| 1:QA:49:U:O4       | 1:QA:365:U:O4      | 2.10                     | 0.69              |
| 13:QM:80:ARG:CB    | 50:R4:71:ARG:HH22  | 2.06                     | 0.69              |
| 51:R5:41:PRO:O     | 51:R5:44:THR:OG1   | 2.10                     | 0.69              |
| 36:RQ:37:LEU:HD21  | 36:RQ:130:LYS:HE3  | 1.74                     | 0.69              |
| 1:XA:674:G:H2'     | 1:XA:675:A:H8      | 1.57                     | 0.69              |
| 13:XM:93:ARG:NH1   | 25:YA:888:C:OP1    | 2.25                     | 0.69              |
| 25:YA:956:G:OP2    | 36:YQ:14:ARG:NH2   | 2.24                     | 0.69              |
| 29:YF:184:TYR:O    | 29:YF:188:ARG:HG3  | 1.93                     | 0.69              |
| 31:RH:86:GLU:HG3   | 31:RH:165:ALA:H    | 1.56                     | 0.69              |
| 1:XA:27:G:H4'      | 4:XD:209:ARG:HG3   | 1.75                     | 0.69              |
| 25:YA:1980:G:O2'   | 25:YA:1982:C:OP2   | 2.09                     | 0.69              |
| 29:YF:110:LEU:HD11 | 29:YF:181:LEU:HD13 | 1.74                     | 0.69              |
| 1:QA:954:G:H21     | 1:QA:1227:A:H62    | 1.40                     | 0.69              |
| 13:QM:57:ARG:NH2   | 50:R4:34:GLU:HA    | 2.08                     | 0.69              |
| 25:RA:2857:G:N2    | 25:RA:2860:A:OP2   | 2.22                     | 0.69              |
| 1:XA:1128:C:N4     | 1:XA:1144:G:H1     | 1.91                     | 0.69              |
| 6:XF:68:PRO:HG2    | 6:XF:71:ARG:HG3    | 1.75                     | 0.69              |
| 28:YE:128:SER:OG   | 28:YE:129:HIS:N    | 2.24                     | 0.69              |
| 19:QS:9:VAL:HG13   | 50:R4:66:SER:O     | 1.94                     | 0.68              |
| 25:RA:1045:A:C6    | 25:RA:1111:A:N7    | 2.61                     | 0.68              |
| 25:RA:2287:A:N6    | 25:RA:2344:U:N3    | 2.35                     | 0.68              |
| 28:RE:2:LYS:HD3    | 28:RE:95:ILE:HG22  | 1.75                     | 0.68              |
| 13:QM:8:GLU:OE1    | 30:RG:115:ARG:CZ   | 2.41                     | 0.68              |
| 32:RI:52:ARG:C     | 32:RI:56:LYS:HB3   | 2.12                     | 0.68              |
| 42:RW:29:LEU:HG    | 42:RW:33:ARG:HD2   | 1.74                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:YZ:141:VAL:HG23 | 45:YZ:144:LEU:HB2 | 1.74                     | 0.68              |
| 27:RD:25:THR:O     | 27:RD:27:THR:N    | 2.26                     | 0.68              |
| 19:XS:3:ARG:HB3    | 50:Y4:67:TYR:HD2  | 1.56                     | 0.68              |
| 29:YF:157:VAL:HB   | 29:YF:194:MET:HB3 | 1.76                     | 0.68              |
| 1:QA:439:A:OP2     | 1:QA:493:G:N1     | 2.26                     | 0.68              |
| 51:R5:55:ARG:HG3   | 51:R5:57:VAL:N    | 2.09                     | 0.68              |
| 45:RZ:110:GLY:HA2  | 45:RZ:111:VAL:C   | 2.14                     | 0.68              |
| 14:YN:13:THR:N     | 14:YN:14:PRO:HD2  | 2.08                     | 0.68              |
| 27:YD:25:THR:O     | 27:YD:27:THR:N    | 2.26                     | 0.68              |
| 39:YT:123:GLN:O    | 39:YT:125:ARG:N   | 2.26                     | 0.68              |
| 1:QA:501:C:OP1     | 12:QL:117:ARG:NH2 | 2.24                     | 0.68              |
| 5:QE:79:GLU:OE2    | 8:QH:104:ARG:HA   | 1.94                     | 0.68              |
| 25:RA:273:G:H1     | 25:RA:364:C:N4    | 1.90                     | 0.68              |
| 30:RG:66:GLN:NE2   | 30:RG:93:THR:O    | 2.26                     | 0.68              |
| 1:XA:992:U:H3      | 1:XA:1044:A:H62   | 1.41                     | 0.68              |
| 1:XA:501:C:OP1     | 12:XL:117:ARG:NH2 | 2.27                     | 0.68              |
| 47:Y1:73:LEU:HD13  | 47:Y1:90:ILE:HG22 | 1.76                     | 0.68              |
| 25:YA:1728:G:N1    | 25:YA:1730:U:OP2  | 2.27                     | 0.68              |
| 25:YA:2123:G:H1    | 25:YA:2175:C:H42  | 1.42                     | 0.68              |
| 25:YA:910:A:H62    | 36:YQ:12:GLN:HA   | 1.57                     | 0.68              |
| 3:QC:3:ASN:N       | 3:QC:3:ASN:OD1    | 2.27                     | 0.68              |
| 23:QW:7:A:H61      | 23:QW:66:U:H3     | 1.42                     | 0.68              |
| 30:RG:47:LYS:HD3   | 30:RG:81:LYS:HB2  | 1.76                     | 0.68              |
| 1:XA:707:C:OP1     | 11:XK:85:ARG:NH1  | 2.26                     | 0.68              |
| 25:YA:2576:G:O2'   | 25:YA:2579:C:OP2  | 2.12                     | 0.68              |
| 35:YP:64:LYS:C     | 35:YP:66:GLY:H    | 1.95                     | 0.68              |
| 25:RA:2131:G:H4'   | 25:RA:2132:U:H4'  | 1.74                     | 0.68              |
| 25:RA:242:G:H5''   | 54:R8:62:LEU:HD13 | 1.74                     | 0.68              |
| 37:RR:38:VAL:HG22  | 37:RR:112:ALA:HB2 | 1.75                     | 0.68              |
| 2:XB:235:SER:OG    | 2:XB:236:TYR:N    | 2.25                     | 0.68              |
| 25:RA:1689:A:H62   | 25:RA:1698:A:H2   | 1.42                     | 0.68              |
| 25:RA:654(A):G:H1  | 25:RA:654(T):C:N4 | 1.91                     | 0.68              |
| 25:RA:978:G:H1     | 25:RA:985:C:N4    | 1.92                     | 0.68              |
| 1:XA:1028(B):C:N4  | 1:XA:1032(A):G:H1 | 1.91                     | 0.68              |
| 1:XA:438:G:H4'     | 4:XD:123:HIS:CD2  | 2.29                     | 0.68              |
| 2:XB:178:ARG:HG3   | 8:XH:72:PRO:HA    | 1.75                     | 0.68              |
| 28:YE:95:ILE:H     | 28:YE:95:ILE:HD12 | 1.59                     | 0.68              |
| 25:YA:2306:C:H3'   | 25:YA:2307:G:H5'' | 1.75                     | 0.68              |
| 27:YD:142:VAL:HG23 | 27:YD:193:VAL:HA  | 1.75                     | 0.68              |
| 31:YH:15:VAL:HG11  | 31:YH:79:VAL:HG23 | 1.75                     | 0.68              |
| 33:YN:133:GLN:HB2  | 33:YN:135:PRO:HD3 | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:37:LEU:HD21 | 36:YQ:130:LYS:HE3 | 1.74                     | 0.68              |
| 1:QA:542:G:OP1    | 4:QD:10:ARG:NH2   | 2.27                     | 0.68              |
| 2:QB:27:LYS:HD2   | 2:QB:193:ASP:HB2  | 1.75                     | 0.68              |
| 36:RQ:12:GLN:HG2  | 36:RQ:73:PRO:HD2  | 1.75                     | 0.68              |
| 5:QE:11:ILE:HG13  | 5:QE:31:LEU:HB3   | 1.76                     | 0.68              |
| 25:YA:573:G:OP2   | 41:YV:78:LYS:NZ   | 2.27                     | 0.68              |
| 27:YD:248:SER:OG  | 27:YD:252:TRP:CE2 | 2.46                     | 0.68              |
| 27:YD:248:SER:OG  | 27:YD:252:TRP:NE1 | 2.25                     | 0.68              |
| 35:YP:39:LYS:HG3  | 35:YP:45:LEU:HD22 | 1.75                     | 0.68              |
| 11:QK:58:PRO:HB2  | 11:QK:93:GLN:HG3  | 1.75                     | 0.67              |
| 22:QV:76:A:HO2'   | 25:RA:2451:A:HO2' | 1.36                     | 0.67              |
| 30:RG:83:ARG:H    | 30:RG:86:MET:HG3  | 1.59                     | 0.67              |
| 1:XA:347:G:H1'    | 1:XA:348:G:H5''   | 1.76                     | 0.67              |
| 25:YA:1509:C:N3   | 25:YA:1511:A:N6   | 2.41                     | 0.67              |
| 26:YB:24:G:O6     | 26:YB:56:G:O2'    | 2.09                     | 0.67              |
| 16:QP:4:ILE:HG12  | 16:QP:21:VAL:HG12 | 1.75                     | 0.67              |
| 25:RA:2115:G:N2   | 25:RA:2165:G:N7   | 2.36                     | 0.67              |
| 13:XM:61:GLU:O    | 50:Y4:49:PHE:CE2  | 2.47                     | 0.67              |
| 25:YA:1021:A:OP2  | 33:YN:65:LYS:NZ   | 2.27                     | 0.67              |
| 1:QA:1346:A:H5''  | 9:QI:120:ARG:HH12 | 1.58                     | 0.67              |
| 19:QS:70:LYS:HZ1  | 50:R4:68:ARG:NH2  | 1.92                     | 0.67              |
| 25:RA:587:C:OP2   | 35:RP:21:ARG:NH2  | 2.28                     | 0.67              |
| 31:RH:127:GLU:HB2 | 31:RH:130:ARG:HB3 | 1.76                     | 0.67              |
| 31:RH:152:ARG:HG3 | 31:RH:153:LYS:HD2 | 1.77                     | 0.67              |
| 54:Y8:29:LYS:O    | 54:Y8:31:HIS:N    | 2.27                     | 0.67              |
| 36:YQ:134:ARG:NH1 | 45:YZ:122:ARG:NH2 | 2.34                     | 0.67              |
| 6:QF:15:ASP:OD2   | 6:QF:18:GLN:CD    | 2.33                     | 0.67              |
| 19:QS:29:ARG:HD3  | 19:QS:30:LEU:HD13 | 1.77                     | 0.67              |
| 51:R5:35:GLU:CB   | 51:R5:49:CYS:SG   | 2.82                     | 0.67              |
| 25:YA:1479:G:N7   | 25:YA:1510:A:N6   | 2.41                     | 0.67              |
| 28:RE:20:ALA:C    | 28:RE:21:VAL:CG1  | 2.62                     | 0.67              |
| 25:RA:1187:G:H5'' | 41:RV:81:TYR:CE1  | 2.29                     | 0.67              |
| 5:XE:31:LEU:HD23  | 5:XE:45:PHE:CD1   | 2.30                     | 0.67              |
| 19:XS:5:LEU:CD1   | 50:Y4:66:SER:HB2  | 2.24                     | 0.67              |
| 25:YA:2308:G:H1   | 25:YA:2311:A:H2   | 1.38                     | 0.67              |
| 25:YA:67:U:N3     | 25:YA:74:A:H2     | 1.92                     | 0.67              |
| 28:YE:1:MET:N     | 28:YE:83:ASP:O    | 2.28                     | 0.67              |
| 31:YH:137:ASP:OD1 | 31:YH:138:LYS:N   | 2.27                     | 0.67              |
| 41:RV:72:VAL:HG13 | 41:RV:85:LYS:HB3  | 1.75                     | 0.67              |
| 19:XS:40:ILE:HG12 | 19:XS:41:VAL:HG13 | 1.76                     | 0.67              |
| 25:YA:2168:G:N2   | 25:YA:2170:A:N7   | 2.42                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:89:ASN:O    | 36:YQ:92:GLY:N    | 2.18                     | 0.67              |
| 25:RA:2168:G:N2   | 25:RA:2170:A:N7   | 2.38                     | 0.67              |
| 25:RA:807:U:H2'   | 25:RA:808:G:H8    | 1.60                     | 0.67              |
| 27:RD:182:LEU:H   | 27:RD:272:ALA:HB3 | 1.59                     | 0.67              |
| 23:XW:49:C:N4     | 23:XW:65:G:H1     | 1.93                     | 0.67              |
| 51:Y5:39:MET:O    | 51:Y5:40:LYS:HG3  | 1.94                     | 0.67              |
| 25:YA:443:A:H3'   | 29:YF:45:ARG:HH12 | 1.60                     | 0.67              |
| 27:YD:35:LYS:HG2  | 27:YD:64:ILE:H    | 1.59                     | 0.67              |
| 25:YA:1490:A:O2'  | 27:YD:99:ASP:OD1  | 2.12                     | 0.67              |
| 35:YP:64:LYS:C    | 35:YP:66:GLY:N    | 2.48                     | 0.67              |
| 1:QA:78:G:O6      | 1:QA:91:C:N4      | 2.27                     | 0.67              |
| 25:RA:857:C:OP2   | 46:R0:77:ARG:NH2  | 2.23                     | 0.67              |
| 39:RT:84:GLN:HG2  | 39:RT:85:LYS:HG2  | 1.76                     | 0.67              |
| 2:XB:174:VAL:HG13 | 2:XB:184:VAL:HG11 | 1.75                     | 0.67              |
| 8:XH:120:THR:H    | 8:XH:123:GLU:HB2  | 1.59                     | 0.67              |
| 26:YB:44:G:H1'    | 26:YB:47:C:N4     | 2.09                     | 0.67              |
| 39:YT:16:ARG:NH2  | 39:YT:83:ILE:O    | 2.27                     | 0.67              |
| 25:RA:49:A:N7     | 25:RA:120:U:C5    | 2.63                     | 0.67              |
| 25:RA:598:G:H5'   | 35:RP:11:GLY:HA3  | 1.77                     | 0.67              |
| 29:RF:143:ALA:HB1 | 29:RF:148:LEU:HB2 | 1.75                     | 0.67              |
| 31:RH:41:MET:HE1  | 31:RH:64:LEU:HD22 | 1.75                     | 0.67              |
| 1:XA:255:G:C6     | 1:XA:256:U:C4     | 2.82                     | 0.67              |
| 1:XA:542:G:OP1    | 4:XD:10:ARG:NH2   | 2.28                     | 0.67              |
| 2:XB:168:THR:HB   | 2:XB:192:SER:HB2  | 1.77                     | 0.67              |
| 32:YI:5:LEU:HD21  | 32:YI:12:LEU:HB3  | 1.76                     | 0.67              |
| 37:YR:78:LYS:HE2  | 37:YR:83:ILE:HD11 | 1.77                     | 0.67              |
| 41:YV:52:VAL:HG21 | 41:YV:55:ALA:HB3  | 1.76                     | 0.67              |
| 1:QA:1347:G:N2    | 1:QA:1374:A:OP2   | 2.26                     | 0.67              |
| 13:QM:57:ARG:HH21 | 50:R4:34:GLU:HA   | 1.58                     | 0.67              |
| 25:RA:2392:A:C8   | 35:RP:60:MET:HG2  | 2.30                     | 0.67              |
| 27:RD:49:ILE:HD11 | 27:RD:52:ARG:HA   | 1.77                     | 0.67              |
| 39:RT:36:GLU:HG3  | 39:RT:41:ARG:HD3  | 1.77                     | 0.67              |
| 7:XG:89:MET:HE1   | 7:XG:156:TRP:H    | 1.60                     | 0.67              |
| 23:XW:38:A:H3'    | 23:XW:39:U:H5''   | 1.77                     | 0.67              |
| 25:YA:1057:A:H62  | 25:YA:1086:A:H2'  | 1.59                     | 0.67              |
| 25:YA:2849:U:H5   | 39:YT:93:ARG:HH12 | 1.42                     | 0.67              |
| 32:RI:3:VAL:HG12  | 32:RI:38:LEU:HA   | 1.77                     | 0.66              |
| 36:RQ:30:GLY:HA2  | 36:RQ:107:ALA:HB2 | 1.78                     | 0.66              |
| 25:YA:2444:G:OP2  | 29:YF:68:LYS:HE3  | 1.94                     | 0.66              |
| 25:RA:654(A):G:N2 | 25:RA:654(T):C:N3 | 2.44                     | 0.66              |
| 32:YI:4:ILE:HG12  | 32:YI:18:VAL:HG22 | 1.76                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:QD:154:ASN:OD1   | 4:QD:154:ASN:N    | 2.26                     | 0.66              |
| 51:R5:58:LEU:HD13  | 51:R5:60:VAL:CG1  | 2.24                     | 0.66              |
| 55:R9:27:CYS:SG    | 55:R9:29:ASN:ND2  | 2.69                     | 0.66              |
| 32:RI:4:ILE:HG12   | 32:RI:18:VAL:HG22 | 1.78                     | 0.66              |
| 1:XA:1028(B):C:H42 | 1:XA:1032(A):G:H1 | 1.43                     | 0.66              |
| 25:YA:581:C:H2'    | 25:YA:582:G:H8    | 1.60                     | 0.66              |
| 51:R5:46:CYS:SG    | 51:R5:49:CYS:N    | 2.61                     | 0.66              |
| 51:R5:56:LYS:HE2   | 51:R5:58:LEU:HD21 | 1.78                     | 0.66              |
| 25:RA:270(R):G:OP1 | 32:RI:42:SER:OG   | 2.12                     | 0.66              |
| 1:XA:1004:A:H1'    | 1:XA:1036:G:H22   | 1.59                     | 0.66              |
| 5:XE:37:ARG:HA     | 5:XE:114:GLY:H    | 1.59                     | 0.66              |
| 10:XJ:7:LYS:HB2    | 10:XJ:97:GLU:HB2  | 1.76                     | 0.66              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:N   | 2.10                     | 0.66              |
| 1:QA:1054:C:OP2    | 1:QA:1197:G:OP2   | 2.14                     | 0.66              |
| 26:RB:24:G:O6      | 26:RB:56:G:O2'    | 2.12                     | 0.66              |
| 30:RG:6:ALA:H      | 50:R4:23:GLU:HG2  | 1.60                     | 0.66              |
| 25:RA:2392:A:H8    | 35:RP:60:MET:HG2  | 1.59                     | 0.66              |
| 1:XA:1053:G:H5'    | 1:XA:1054:C:H5'   | 1.77                     | 0.66              |
| 13:XM:105:THR:O    | 13:XM:107:ALA:N   | 2.29                     | 0.66              |
| 25:YA:674:G:H1'    | 29:YF:74:ARG:HD3  | 1.77                     | 0.66              |
| 42:YW:45:TYR:CZ    | 42:YW:49:LYS:HD2  | 2.30                     | 0.66              |
| 44:YY:49:VAL:O     | 44:YY:51:VAL:N    | 2.29                     | 0.66              |
| 3:QC:70:VAL:HG12   | 3:QC:72:LYS:H     | 1.60                     | 0.66              |
| 1:QA:8:A:N6        | 4:QD:205:GLU:O    | 2.28                     | 0.66              |
| 47:R1:7:ILE:HG12   | 47:R1:91:LYS:NZ   | 2.11                     | 0.66              |
| 25:YA:1407:C:H42   | 25:YA:1595:G:H1   | 1.43                     | 0.66              |
| 44:YY:97:ARG:HE    | 44:YY:98:VAL:HB   | 1.61                     | 0.66              |
| 36:YQ:137:TYR:CE1  | 45:YZ:83:PRO:HG3  | 2.31                     | 0.66              |
| 13:QM:80:ARG:HE    | 50:R4:71:ARG:NH1  | 1.87                     | 0.66              |
| 19:QS:39:THR:HG22  | 19:QS:40:ILE:H    | 1.61                     | 0.66              |
| 25:RA:2298:A:H62   | 25:RA:2318:G:H8   | 1.44                     | 0.66              |
| 25:RA:372:G:N2     | 25:RA:401:A:OP2   | 2.23                     | 0.66              |
| 28:RE:63:LEU:HD13  | 28:RE:65:GLY:H    | 1.60                     | 0.66              |
| 25:YA:2343:C:O2'   | 25:YA:2373:G:O2'  | 2.14                     | 0.66              |
| 1:QA:1002:G:H2'    | 1:QA:1003:G:C8    | 2.30                     | 0.66              |
| 29:RF:149:ASP:N    | 29:RF:149:ASP:OD1 | 2.27                     | 0.66              |
| 25:YA:2470:G:H5'   | 36:YQ:56:ARG:HH22 | 1.61                     | 0.66              |
| 45:YZ:182:LYS:HG3  | 45:YZ:183:LEU:HA  | 1.78                     | 0.66              |
| 45:YZ:60:GLU:HA    | 45:YZ:66:SER:HA   | 1.77                     | 0.66              |
| 1:QA:1055:A:O2'    | 3:QC:161:GLU:OE2  | 2.12                     | 0.66              |
| 25:YA:1013:C:H42   | 25:YA:1149:G:H1   | 1.43                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:780:G:N2    | 25:YA:783:A:H62    | 1.94                     | 0.66              |
| 33:YN:35:ARG:O    | 33:YN:37:LYS:N     | 2.29                     | 0.66              |
| 35:YP:105:LEU:O   | 35:YP:106:LEU:HB2  | 1.95                     | 0.66              |
| 38:YS:55:ALA:O    | 38:YS:56:LEU:HB2   | 1.96                     | 0.66              |
| 45:YZ:128:VAL:HB  | 45:YZ:161:VAL:HG13 | 1.77                     | 0.66              |
| 1:QA:1175:G:H2'   | 1:QA:1176:A:C8     | 2.30                     | 0.66              |
| 36:RQ:135:ASP:OD1 | 36:RQ:135:ASP:N    | 2.23                     | 0.66              |
| 44:RY:49:VAL:O    | 44:RY:51:VAL:N     | 2.29                     | 0.66              |
| 45:RZ:19:ARG:NH1  | 45:RZ:84:GLU:O     | 2.28                     | 0.66              |
| 19:XS:50:ALA:HB1  | 19:XS:57:HIS:HB3   | 1.77                     | 0.66              |
| 25:YA:2848:G:O2'  | 25:YA:2867:G:N2    | 2.28                     | 0.66              |
| 41:YV:21:ARG:HD2  | 41:YV:91:TYR:CD1   | 2.31                     | 0.66              |
| 39:RT:102:ILE:HB  | 39:RT:110:ILE:HD13 | 1.78                     | 0.65              |
| 25:YA:2051:A:H2   | 25:YA:2052:G:O6    | 1.76                     | 0.65              |
| 31:YH:153:LYS:HB3 | 31:YH:162:ILE:H    | 1.61                     | 0.65              |
| 39:YT:16:ARG:HD3  | 39:YT:19:LEU:HD11  | 1.77                     | 0.65              |
| 50:R4:1:MET:SD    | 50:R4:6:HIS:NE2    | 2.69                     | 0.65              |
| 51:R5:58:LEU:H    | 51:R5:58:LEU:HD12  | 1.59                     | 0.65              |
| 53:R7:9:ARG:HH21  | 53:R7:48:LYS:CD    | 1.99                     | 0.65              |
| 25:RA:1359:A:N1   | 25:RA:1372:U:C4    | 2.64                     | 0.65              |
| 25:RA:2747:G:H21  | 25:RA:2757:A:H62   | 1.43                     | 0.65              |
| 43:RX:60:ARG:HH12 | 53:R7:47:ARG:HH22  | 1.40                     | 0.65              |
| 1:XA:1305:G:N2    | 1:XA:1331:G:H2'    | 2.11                     | 0.65              |
| 1:XA:555:C:OP2    | 12:XL:20:LYS:NZ    | 2.29                     | 0.65              |
| 47:Y1:29:GLY:O    | 47:Y1:31:GLY:N     | 2.30                     | 0.65              |
| 31:YH:10:PRO:HD2  | 31:YH:50:VAL:HG13  | 1.78                     | 0.65              |
| 1:QA:1296:C:OP1   | 13:QM:44:ARG:NH2   | 2.29                     | 0.65              |
| 27:RD:108:PRO:HG2 | 27:RD:111:LEU:HG   | 1.78                     | 0.65              |
| 27:RD:27:THR:HG21 | 27:RD:81:ALA:HB1   | 1.78                     | 0.65              |
| 31:RH:125:VAL:CB  | 31:RH:126:PRO:HD3  | 2.16                     | 0.65              |
| 31:RH:89:ILE:CD1  | 31:RH:129:THR:HB   | 2.27                     | 0.65              |
| 25:RA:483:A:H4'   | 44:RY:49:VAL:HA    | 1.78                     | 0.65              |
| 25:YA:1568:G:H4'  | 27:YD:59:LYS:HB3   | 1.78                     | 0.65              |
| 25:YA:443:A:H3'   | 29:YF:45:ARG:NH1   | 2.11                     | 0.65              |
| 1:QA:1298:C:OP2   | 7:QG:114:ARG:NH2   | 2.30                     | 0.65              |
| 1:QA:191:G:H1'    | 20:QT:105:SER:HB3  | 1.77                     | 0.65              |
| 52:R6:11:LEU:HD23 | 52:R6:26:ASN:HB3   | 1.78                     | 0.65              |
| 35:RP:59:LEU:HA   | 35:RP:61:ARG:NE    | 2.12                     | 0.65              |
| 35:YP:61:ARG:HD3  | 54:Y8:13:ARG:HD2   | 1.77                     | 0.65              |
| 25:YA:1077:A:H5'  | 25:YA:1078:U:H5''  | 1.77                     | 0.65              |
| 25:YA:2023:G:H5'  | 25:YA:2617:C:H4'   | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:YU:8:VAL:HG23   | 40:YU:11:ARG:HH21  | 1.62                     | 0.65              |
| 45:RZ:150:LEU:HD21 | 45:RZ:172:ALA:HB3  | 1.77                     | 0.65              |
| 1:XA:1525:G:OP1    | 11:XK:120:ARG:NH2  | 2.30                     | 0.65              |
| 25:YA:793:A:OP2    | 25:YA:2071:A:O2'   | 2.15                     | 0.65              |
| 2:QB:82:ARG:HA     | 2:QB:92:TYR:CE2    | 2.31                     | 0.65              |
| 25:RA:224:G:O6     | 25:RA:419:C:O2'    | 2.15                     | 0.65              |
| 44:RY:38:ILE:HG22  | 44:RY:66:PRO:HA    | 1.79                     | 0.65              |
| 48:Y2:50:ILE:HD12  | 48:Y2:51:ARG:H     | 1.62                     | 0.65              |
| 25:YA:1754:C:OP1   | 39:YT:96:ARG:NH1   | 2.29                     | 0.65              |
| 51:R5:49:CYS:O     | 51:R5:56:LYS:HD3   | 1.96                     | 0.65              |
| 25:YA:2502:G:H5''  | 25:YA:2503:A:H5''  | 1.79                     | 0.65              |
| 31:YH:20:ALA:HB3   | 31:YH:23:ARG:HG2   | 1.77                     | 0.65              |
| 25:RA:504:U:H5''   | 25:RA:505:A:H5'    | 1.78                     | 0.65              |
| 25:RA:27:G:N2      | 25:RA:513:A:OP2    | 2.29                     | 0.65              |
| 28:RE:14:ILE:O     | 28:RE:21:VAL:N     | 2.28                     | 0.65              |
| 35:RP:71:VAL:HG13  | 35:RP:72:PRO:HD3   | 1.78                     | 0.65              |
| 1:XA:1002:G:H2'    | 1:XA:1003:G:H8     | 1.61                     | 0.65              |
| 1:XA:191:G:O2'     | 20:XT:101:GLY:O    | 2.15                     | 0.65              |
| 20:XT:97:ALA:O     | 20:XT:99:LEU:N     | 2.30                     | 0.65              |
| 46:Y0:10:THR:HG22  | 46:Y0:12:ASN:H     | 1.62                     | 0.65              |
| 25:YA:128:C:H4'    | 53:Y7:49:ARG:HH12  | 1.61                     | 0.65              |
| 3:QC:9:GLY:HA2     | 3:QC:12:LEU:HD23   | 1.78                     | 0.65              |
| 16:QP:53:VAL:HG12  | 16:QP:79:VAL:HG22  | 1.77                     | 0.65              |
| 35:RP:47:ASP:OD2   | 35:RP:50:ARG:NH2   | 2.30                     | 0.65              |
| 1:XA:1014:A:H4'    | 19:XS:14:HIS:CD2   | 2.31                     | 0.65              |
| 11:XK:21:ILE:HB    | 11:XK:84:VAL:HG12  | 1.78                     | 0.65              |
| 51:Y5:56:LYS:HD2   | 51:Y5:56:LYS:H     | 1.60                     | 0.65              |
| 32:YI:40:THR:O     | 32:YI:44:LEU:HB2   | 1.97                     | 0.65              |
| 13:QM:3:ARG:HD2    | 13:QM:9:ILE:HG12   | 1.79                     | 0.65              |
| 25:RA:2701:C:H3'   | 25:RA:2702:U:C5'   | 2.23                     | 0.65              |
| 25:RA:819:A:OP2    | 25:RA:1187:G:N2    | 2.24                     | 0.65              |
| 29:RF:31:HIS:HB2   | 35:RP:9:ASN:OD1    | 1.96                     | 0.65              |
| 2:XB:178:ARG:NH1   | 2:XB:196:LEU:O     | 2.29                     | 0.65              |
| 25:YA:855:G:O2'    | 46:Y0:27:GLU:OE2   | 2.10                     | 0.65              |
| 51:Y5:4:HIS:HB3    | 51:Y5:5:PRO:HD3    | 1.79                     | 0.65              |
| 27:YD:30:GLU:HG3   | 27:YD:63:ARG:NH2   | 2.12                     | 0.65              |
| 27:YD:80:ALA:HB3   | 27:YD:94:LEU:HD13  | 1.79                     | 0.65              |
| 51:R5:50:GLY:CA    | 51:R5:56:LYS:HB3   | 2.22                     | 0.64              |
| 34:RO:4:PRO:O      | 34:RO:5:GLN:HB2    | 1.96                     | 0.64              |
| 1:XA:1405:G:OP2    | 58:XA:1672:PAR:O34 | 2.15                     | 0.64              |
| 3:XC:122:GLU:OE1   | 3:XC:126:ARG:NH2   | 2.29                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:XD:9:CYS:SG     | 4:XD:31:CYS:O     | 2.54                     | 0.64              |
| 25:YA:2404:C:O3'  | 35:YP:77:ARG:NH2  | 2.29                     | 0.64              |
| 25:YA:607:U:H3    | 25:YA:621:A:H2    | 1.42                     | 0.64              |
| 29:YF:107:LYS:HD2 | 29:YF:207:GLY:H   | 1.62                     | 0.64              |
| 19:QS:28:LYS:HB2  | 19:QS:47:HIS:CE1  | 2.32                     | 0.64              |
| 19:QS:67:VAL:HG11 | 50:R4:59:PHE:O    | 1.98                     | 0.64              |
| 25:RA:2693:A:H2'  | 25:RA:2694:G:H8   | 1.62                     | 0.64              |
| 27:RD:35:LYS:HG2  | 27:RD:64:ILE:N    | 2.12                     | 0.64              |
| 35:RP:85:LEU:HA   | 35:RP:88:LEU:HD22 | 1.79                     | 0.64              |
| 25:YA:819:A:OP2   | 25:YA:1187:G:N2   | 2.23                     | 0.64              |
| 27:YD:44:ASN:HB3  | 27:YD:49:ILE:HA   | 1.78                     | 0.64              |
| 1:QA:1227:A:OP1   | 19:QS:80:TYR:OH   | 2.12                     | 0.64              |
| 25:RA:489:G:N7    | 42:RW:49:LYS:NZ   | 2.46                     | 0.64              |
| 25:RA:2683:C:OP1  | 39:RT:53:ARG:NH2  | 2.30                     | 0.64              |
| 13:XM:3:ARG:HB3   | 50:Y4:34:GLU:HB3  | 1.79                     | 0.64              |
| 25:YA:1055:G:H1   | 25:YA:1104:C:H42  | 1.44                     | 0.64              |
| 5:QE:11:ILE:HD11  | 5:QE:31:LEU:HD12  | 1.80                     | 0.64              |
| 10:QJ:53:PRO:HA   | 14:QN:42:ILE:HD12 | 1.79                     | 0.64              |
| 13:QM:121:LYS:NZ  | 23:QY:40:C:O2'    | 2.29                     | 0.64              |
| 51:R5:58:LEU:O    | 51:R5:60:VAL:N    | 2.31                     | 0.64              |
| 27:RD:65:ILE:HD11 | 27:RD:67:PHE:CE2  | 2.31                     | 0.64              |
| 27:RD:8:PRO:HB3   | 27:RD:14:ARG:HB2  | 1.79                     | 0.64              |
| 28:RE:21:VAL:CB   | 28:RE:22:PRO:HA   | 2.28                     | 0.64              |
| 1:XA:1321:C:H3'   | 1:XA:1322:C:H5''  | 1.80                     | 0.64              |
| 23:XW:50:U:O4     | 23:XW:64:A:N1     | 2.30                     | 0.64              |
| 36:YQ:78:PRO:O    | 36:YQ:79:LEU:HB2  | 1.97                     | 0.64              |
| 1:QA:664:G:H22    | 1:QA:741:G:H1     | 1.45                     | 0.64              |
| 25:RA:141:A:H8    | 25:RA:1595:G:H21  | 1.46                     | 0.64              |
| 15:XO:26:GLU:OE2  | 15:XO:77:ARG:NH1  | 2.31                     | 0.64              |
| 38:YS:58:LEU:CD2  | 38:YS:58:LEU:H    | 2.10                     | 0.64              |
| 25:RA:2114:A:N6   | 25:RA:2119:A:N7   | 2.46                     | 0.64              |
| 36:RQ:17:LEU:HD21 | 36:RQ:41:TRP:CD1  | 2.33                     | 0.64              |
| 40:RU:90:VAL:O    | 40:RU:92:ARG:N    | 2.30                     | 0.64              |
| 25:YA:690:G:O2'   | 27:YD:43:ARG:NH2  | 2.30                     | 0.64              |
| 40:YU:88:ILE:HG22 | 40:YU:90:VAL:HG23 | 1.79                     | 0.64              |
| 27:RD:35:LYS:HG2  | 27:RD:64:ILE:H    | 1.63                     | 0.64              |
| 25:RA:2636:U:OP1  | 28:RE:79:ARG:HA   | 1.97                     | 0.64              |
| 13:XM:54:VAL:HG23 | 50:Y4:32:TYR:HH   | 1.59                     | 0.64              |
| 45:YZ:93:ASP:C    | 45:YZ:94:GLU:HG2  | 2.10                     | 0.64              |
| 45:YZ:91:LEU:HD11 | 45:YZ:96:VAL:HG21 | 1.79                     | 0.64              |
| 1:QA:963:G:H1     | 1:QA:972:C:N4     | 1.92                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:QB:5:ILE:HG21    | 2:QB:221:LEU:HD23 | 1.78                     | 0.64              |
| 25:RA:1543:A:C2    | 25:RA:1545:A:C8   | 2.86                     | 0.64              |
| 25:RA:2100:G:H1    | 25:RA:2189:U:H3   | 1.44                     | 0.64              |
| 29:RF:192:LEU:HD22 | 29:RF:194:MET:HG2 | 1.80                     | 0.64              |
| 25:RA:2547:U:O2    | 34:RO:23:ARG:NH2  | 2.31                     | 0.64              |
| 4:QD:194:LEU:CD1   | 6:XF:17:SER:OG    | 2.46                     | 0.64              |
| 26:YB:52:A:H62     | 38:YS:33:LYS:HG3  | 1.63                     | 0.64              |
| 37:YR:51:LEU:HD13  | 37:YR:66:VAL:HG13 | 1.79                     | 0.64              |
| 39:YT:36:GLU:HG3   | 39:YT:41:ARG:HE   | 1.62                     | 0.64              |
| 1:QA:1128:C:OP1    | 9:QI:66:ARG:NH2   | 2.26                     | 0.64              |
| 1:QA:963:G:N2      | 1:QA:972:C:N3     | 2.40                     | 0.64              |
| 10:QJ:77:PRO:O     | 10:QJ:79:ARG:NH1  | 2.30                     | 0.64              |
| 36:RQ:83:MET:HB2   | 46:R0:7:LEU:HD12  | 1.78                     | 0.64              |
| 50:R4:48:ARG:O     | 50:R4:50:VAL:N    | 2.31                     | 0.64              |
| 25:RA:517:C:OP1    | 51:R5:16:ARG:NH2  | 2.31                     | 0.64              |
| 31:RH:88:LEU:HD11  | 31:RH:165:ALA:HB2 | 1.80                     | 0.64              |
| 35:RP:10:PRO:O     | 35:RP:12:ALA:N    | 2.30                     | 0.64              |
| 1:XA:1352:C:H42    | 1:XA:1370:G:H1    | 1.46                     | 0.64              |
| 3:XC:11:ARG:O      | 3:XC:13:GLY:N     | 2.30                     | 0.64              |
| 3:XC:19:GLU:O      | 3:XC:40:ARG:NH2   | 2.30                     | 0.64              |
| 5:XE:98:THR:HB     | 5:XE:117:ASP:HB3  | 1.79                     | 0.64              |
| 8:XH:7:ALA:HB2     | 8:XH:85:ARG:HD3   | 1.80                     | 0.64              |
| 19:XS:5:LEU:HD11   | 50:Y4:66:SER:CB   | 2.27                     | 0.64              |
| 25:YA:2111:C:N3    | 25:YA:2118:U:O2'  | 2.30                     | 0.64              |
| 25:YA:581:C:H2'    | 25:YA:582:G:C8    | 2.33                     | 0.64              |
| 27:YD:35:LYS:NZ    | 27:YD:64:ILE:O    | 2.31                     | 0.64              |
| 25:YA:2406:U:N3    | 35:YP:73:GLY:O    | 2.24                     | 0.64              |
| 10:QJ:4:ILE:HB     | 10:QJ:74:ILE:HG13 | 1.80                     | 0.63              |
| 25:RA:1059:G:O6    | 25:RA:1079:C:N4   | 2.30                     | 0.63              |
| 38:RS:26:LEU:HB3   | 38:RS:87:PHE:HA   | 1.81                     | 0.63              |
| 43:RX:43:VAL:HG13  | 43:RX:51:VAL:HG21 | 1.79                     | 0.63              |
| 1:XA:186(E):C:H42  | 1:XA:191(B):G:H1  | 1.45                     | 0.63              |
| 30:YG:112:PRO:HB3  | 50:Y4:37:SER:HB2  | 1.80                     | 0.63              |
| 6:QF:15:ASP:OD2    | 6:QF:18:GLN:OE1   | 2.16                     | 0.63              |
| 25:RA:1266:G:O2'   | 25:RA:2012:G:O6   | 2.14                     | 0.63              |
| 25:RA:2848:G:O2'   | 25:RA:2867:G:N2   | 2.31                     | 0.63              |
| 37:RR:104:ARG:HD3  | 37:RR:109:ALA:HB3 | 1.79                     | 0.63              |
| 1:XA:1321:C:H5''   | 1:XA:1322:C:H5''  | 1.79                     | 0.63              |
| 5:XE:147:ASP:O     | 5:XE:151:LEU:HG   | 1.97                     | 0.63              |
| 48:Y2:41:ILE:HD11  | 48:Y2:44:LEU:HG   | 1.80                     | 0.63              |
| 51:Y5:48:GLU:O     | 51:Y5:58:LEU:HA   | 1.97                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1224:G:C6     | 1:QA:1322:C:H1'    | 2.33                     | 0.63              |
| 19:XS:5:LEU:CD1    | 50:Y4:66:SER:CB    | 2.76                     | 0.63              |
| 54:Y8:16:ILE:HD13  | 54:Y8:57:ARG:HG2   | 1.80                     | 0.63              |
| 27:YD:35:LYS:HG2   | 27:YD:64:ILE:N     | 2.13                     | 0.63              |
| 25:RA:2053:G:O6    | 25:RA:2614:A:C2    | 2.41                     | 0.63              |
| 28:RE:21:VAL:CG2   | 28:RE:22:PRO:CA    | 2.76                     | 0.63              |
| 5:XE:152:ARG:NH2   | 8:XH:107:LEU:O     | 2.31                     | 0.63              |
| 19:XS:67:VAL:HG21  | 50:Y4:60:GLN:NE2   | 2.11                     | 0.63              |
| 50:Y4:48:ARG:O     | 50:Y4:50:VAL:N     | 2.31                     | 0.63              |
| 44:YY:91:GLU:HG3   | 44:YY:92:ASN:H     | 1.63                     | 0.63              |
| 1:QA:243:A:H4'     | 1:QA:244:U:O5'     | 1.98                     | 0.63              |
| 47:R1:29:GLY:O     | 47:R1:31:GLY:N     | 2.29                     | 0.63              |
| 25:RA:2849:U:OP1   | 39:RT:95:ARG:NH1   | 2.30                     | 0.63              |
| 45:RZ:165:VAL:HG11 | 45:RZ:169:GLU:HB2  | 1.80                     | 0.63              |
| 2:XB:187:LEU:HA    | 2:XB:201:ILE:HB    | 1.79                     | 0.63              |
| 13:XM:3:ARG:NH2    | 30:YG:139:LEU:HD13 | 2.12                     | 0.63              |
| 25:YA:2126:A:N6    | 25:YA:2163:C:O2'   | 2.31                     | 0.63              |
| 25:YA:224:G:O6     | 25:YA:419:C:O2'    | 2.17                     | 0.63              |
| 27:YD:25:THR:HG23  | 27:YD:27:THR:HB    | 1.80                     | 0.63              |
| 31:YH:12:PRO:O     | 31:YH:13:LYS:HB2   | 1.97                     | 0.63              |
| 35:YP:13:ASN:O     | 35:YP:15:ARG:N     | 2.32                     | 0.63              |
| 1:QA:1080:A:H5''   | 5:QE:16:THR:HG21   | 1.81                     | 0.63              |
| 19:QS:42:PRO:HD3   | 50:R4:63:TYR:CZ    | 2.33                     | 0.63              |
| 48:R2:65:ASN:HB3   | 48:R2:69:ARG:HH22  | 1.61                     | 0.63              |
| 25:RA:2511:U:O4    | 25:RA:2575:C:N3    | 2.32                     | 0.63              |
| 25:RA:309:G:N3     | 25:RA:329:G:O2'    | 2.31                     | 0.63              |
| 37:RR:33:ARG:HG3   | 37:RR:115:GLU:HB3  | 1.79                     | 0.63              |
| 40:RU:66:ASN:O     | 40:RU:70:ARG:HB2   | 1.98                     | 0.63              |
| 1:XA:1028(B):C:N3  | 1:XA:1032(A):G:N2  | 2.45                     | 0.63              |
| 2:XB:79:ASP:HA     | 2:XB:82:ARG:HB2    | 1.81                     | 0.63              |
| 13:XM:91:ARG:HB2   | 13:XM:98:VAL:HG13  | 1.80                     | 0.63              |
| 25:YA:1918:A:O2'   | 25:YA:1920:C:N4    | 2.32                     | 0.63              |
| 25:YA:2415:G:H4'   | 35:YP:67:MET:N     | 2.14                     | 0.63              |
| 25:RA:2224:G:OP1   | 27:RD:268:ARG:HD3  | 1.98                     | 0.63              |
| 35:RP:95:VAL:HG13  | 35:RP:100:LEU:HD21 | 1.79                     | 0.63              |
| 13:XM:23:TYR:HB3   | 13:XM:67:GLU:HA    | 1.81                     | 0.63              |
| 53:Y7:9:ARG:HH21   | 53:Y7:48:LYS:HD2   | 1.63                     | 0.63              |
| 31:YH:153:LYS:HG3  | 31:YH:161:GLY:HA2  | 1.80                     | 0.63              |
| 31:YH:83:TYR:CZ    | 31:YH:138:LYS:HD2  | 2.34                     | 0.63              |
| 32:YI:56:LYS:HG3   | 32:YI:57:ARG:N     | 2.13                     | 0.63              |
| 1:QA:1002:G:H2'    | 1:QA:1003:G:H8     | 1.61                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:QD:166:LYS:CG   | 4:QD:178:VAL:HG11 | 2.20                     | 0.63              |
| 25:RA:2233:U:H2'  | 25:RA:2234:G:C8   | 2.33                     | 0.63              |
| 25:RA:288:C:H2'   | 25:RA:289:A:H8    | 1.64                     | 0.63              |
| 25:RA:74:A:H4'    | 25:RA:75:G:O5'    | 1.98                     | 0.63              |
| 25:RA:84:A:N1     | 25:RA:98:G:O2'    | 2.31                     | 0.63              |
| 33:RN:133:GLN:HB2 | 33:RN:135:PRO:HD3 | 1.79                     | 0.63              |
| 38:RS:15:ARG:HH11 | 38:RS:25:ARG:HH21 | 1.44                     | 0.63              |
| 1:XA:1106:G:H5''  | 3:XC:172:ARG:HG2  | 1.79                     | 0.63              |
| 1:XA:1298:C:H2'   | 7:XG:114:ARG:NH1  | 2.14                     | 0.63              |
| 9:XI:24:GLY:N     | 9:XI:60:ASP:OD1   | 2.29                     | 0.63              |
| 3:QC:79:ARG:CD    | 11:XK:99:GLN:NE2  | 2.60                     | 0.63              |
| 50:Y4:23:GLU:O    | 50:Y4:25:TYR:N    | 2.31                     | 0.63              |
| 42:YW:41:LYS:HE3  | 51:Y5:25:LEU:HD21 | 1.80                     | 0.63              |
| 52:Y6:41:PRO:HG2  | 52:Y6:45:LYS:H    | 1.63                     | 0.63              |
| 25:YA:2394:C:OP1  | 35:YP:63:PRO:HD2  | 1.99                     | 0.63              |
| 34:YO:13:ASN:ND2  | 34:YO:96:THR:O    | 2.30                     | 0.63              |
| 40:YU:83:LEU:HD12 | 40:YU:113:ALA:HB2 | 1.79                     | 0.63              |
| 1:QA:1446:A:O2'   | 1:QA:1447:G:O5'   | 2.16                     | 0.63              |
| 1:QA:937:A:N6     | 1:QA:1345:U:O4    | 2.30                     | 0.63              |
| 2:QB:24:TRP:HD1   | 2:QB:24:TRP:H     | 1.46                     | 0.63              |
| 8:QH:10:LEU:HD22  | 8:QH:83:ILE:HD11  | 1.80                     | 0.63              |
| 33:RN:13:TRP:HB2  | 33:RN:133:GLN:HG3 | 1.81                     | 0.63              |
| 25:RA:2818:G:OP2  | 37:RR:42:LYS:NZ   | 2.31                     | 0.63              |
| 44:RY:51:VAL:HG13 | 44:RY:52:SER:H    | 1.64                     | 0.63              |
| 25:YA:2310:A:N6   | 30:YG:79:ASN:HB2  | 2.13                     | 0.63              |
| 1:QA:789:U:H1'    | 1:QA:792:A:H2     | 1.64                     | 0.62              |
| 7:QG:155:ARG:HD3  | 7:QG:155:ARG:H    | 1.64                     | 0.62              |
| 11:QK:98:LEU:O    | 11:QK:101:SER:OG  | 2.14                     | 0.62              |
| 25:RA:249:C:O2    | 54:R8:12:LYS:NZ   | 2.32                     | 0.62              |
| 1:XA:1023:G:H3'   | 1:XA:1024:G:H5''  | 1.79                     | 0.62              |
| 1:XA:1446:A:O2'   | 1:XA:1447:G:O5'   | 2.17                     | 0.62              |
| 1:QA:1064:G:O2'   | 1:QA:1065:U:O5'   | 2.17                     | 0.62              |
| 4:QD:7:PRO:HB2    | 4:QD:10:ARG:HD2   | 1.81                     | 0.62              |
| 19:QS:40:ILE:HG23 | 19:QS:41:VAL:HG22 | 1.79                     | 0.62              |
| 25:RA:1311:G:H21  | 25:RA:1603:A:H62  | 1.45                     | 0.62              |
| 25:RA:2306:C:H3'  | 25:RA:2307:G:H5'' | 1.79                     | 0.62              |
| 25:RA:259:G:HO2'  | 25:RA:621:A:HO2'  | 1.47                     | 0.62              |
| 28:RE:15:PHE:CE1  | 28:RE:20:ALA:CB   | 2.82                     | 0.62              |
| 1:XA:1200:C:H4'   | 1:XA:1201:A:H5'   | 1.80                     | 0.62              |
| 10:XJ:32:ALA:HB3  | 10:XJ:76:ASN:HB2  | 1.79                     | 0.62              |
| 25:YA:2789:C:H1'  | 25:YA:2892:A:H2   | 1.64                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:YH:26:VAL:HG11 | 31:YH:75:ALA:HB1   | 1.81                     | 0.62              |
| 1:QA:1135:U:H4'   | 1:QA:1136:U:H5     | 1.64                     | 0.62              |
| 37:RR:33:ARG:HH12 | 51:R5:57:VAL:CG2   | 2.12                     | 0.62              |
| 51:R5:58:LEU:C    | 51:R5:60:VAL:H     | 2.01                     | 0.62              |
| 25:RA:1496:A:H8   | 25:RA:1577:C:HO2'  | 1.47                     | 0.62              |
| 25:RA:2576:G:O2'  | 25:RA:2579:C:OP2   | 2.16                     | 0.62              |
| 25:RA:27:G:H1'    | 25:RA:513:A:N6     | 2.14                     | 0.62              |
| 2:XB:92:TYR:CE1   | 2:XB:151:GLY:HA3   | 2.34                     | 0.62              |
| 2:XB:212:GLN:NE2  | 2:XB:235:SER:HB2   | 2.15                     | 0.62              |
| 1:XA:1455:G:H5'   | 20:XT:31:SER:HB2   | 1.81                     | 0.62              |
| 25:YA:1296:G:OP1  | 25:YA:2709:G:O2'   | 2.13                     | 0.62              |
| 25:YA:1833:U:O2'  | 25:YA:1969:A:N1    | 2.29                     | 0.62              |
| 32:YI:124:GLY:H   | 32:YI:142:VAL:HG23 | 1.63                     | 0.62              |
| 39:YT:1:MET:O     | 39:YT:3:ARG:N      | 2.29                     | 0.62              |
| 28:RE:119:ARG:HG2 | 28:RE:160:TYR:HB2  | 1.81                     | 0.62              |
| 29:RF:12:LEU:HD12 | 29:RF:17:ARG:HG2   | 1.80                     | 0.62              |
| 7:XG:111:ARG:NH1  | 7:XG:113:GLU:OE2   | 2.31                     | 0.62              |
| 19:XS:13:ASP:N    | 19:XS:13:ASP:OD1   | 2.32                     | 0.62              |
| 27:YD:248:SER:CB  | 27:YD:252:TRP:CZ2  | 2.83                     | 0.62              |
| 29:YF:46:ARG:HG2  | 29:YF:46:ARG:HH11  | 1.65                     | 0.62              |
| 30:YG:3:LEU:HD12  | 30:YG:4:ASP:H      | 1.64                     | 0.62              |
| 17:QQ:66:SER:O    | 17:QQ:70:ARG:NH1   | 2.33                     | 0.62              |
| 43:RX:53:LYS:HB2  | 43:RX:82:GLN:HB3   | 1.80                     | 0.62              |
| 10:XJ:5:ARG:HH21  | 10:XJ:99:LYS:HD2   | 1.63                     | 0.62              |
| 1:QA:1163:C:H42   | 1:QA:1173:G:H1     | 1.47                     | 0.62              |
| 6:QF:17:SER:O     | 6:QF:18:GLN:C      | 2.34                     | 0.62              |
| 19:QS:68:GLY:N    | 50:R4:59:PHE:CE1   | 2.67                     | 0.62              |
| 19:QS:68:GLY:CA   | 50:R4:68:ARG:HB2   | 2.28                     | 0.62              |
| 25:RA:2816:C:O3'  | 37:RR:99:LYS:NZ    | 2.33                     | 0.62              |
| 2:XB:54:THR:HG21  | 2:XB:201:ILE:HD11  | 1.82                     | 0.62              |
| 19:XS:5:LEU:HD11  | 50:Y4:66:SER:C     | 2.19                     | 0.62              |
| 28:YE:23:VAL:HG12 | 28:YE:184:VAL:O    | 2.00                     | 0.62              |
| 1:QA:532:A:H2     | 1:QA:1206:G:H21    | 1.46                     | 0.62              |
| 8:QH:6:ILE:HB     | 8:QH:85:ARG:NH1    | 2.15                     | 0.62              |
| 11:QK:121:PRO:HD2 | 11:QK:126:ARG:HD3  | 1.80                     | 0.62              |
| 25:RA:2111:C:N3   | 25:RA:2118:U:O2'   | 2.31                     | 0.62              |
| 25:RA:2133:G:H1'  | 25:RA:2158:A:H61   | 1.64                     | 0.62              |
| 25:RA:996:A:H4'   | 40:RU:92:ARG:HE    | 1.64                     | 0.62              |
| 26:RB:44:G:O2'    | 26:RB:47:C:N4      | 2.31                     | 0.62              |
| 2:XB:12:GLU:O     | 2:XB:16:HIS:ND1    | 2.22                     | 0.62              |
| 13:XM:7:VAL:HG22  | 13:XM:7:VAL:O      | 2.00                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:263:C:H2'    | 25:YA:264:C:O4'    | 2.00                     | 0.62              |
| 32:YI:81:VAL:HG21  | 32:YI:88:ILE:HD12  | 1.80                     | 0.62              |
| 1:QA:448:A:OP2     | 1:QA:485:G:N2      | 2.30                     | 0.62              |
| 3:QC:79:ARG:HH21   | 11:XK:96:ARG:CG    | 2.12                     | 0.62              |
| 1:QA:27:G:H4'      | 4:QD:209:ARG:HG3   | 1.79                     | 0.62              |
| 7:QG:149:ARG:HD3   | 11:QK:59:TYR:OH    | 1.99                     | 0.62              |
| 39:RT:54:ARG:HA    | 39:RT:59:THR:HG23  | 1.82                     | 0.62              |
| 25:YA:1728:G:H8    | 25:YA:1732:A:H62   | 1.48                     | 0.62              |
| 25:YA:1754:C:P     | 39:YT:96:ARG:HH12  | 2.21                     | 0.62              |
| 22:QV:53:G:H4'     | 22:QV:54:U:OP1     | 1.99                     | 0.62              |
| 25:RA:221:A:H4'    | 25:RA:222:A:O5'    | 1.98                     | 0.62              |
| 27:RD:35:LYS:HD2   | 27:RD:104:TYR:CD1  | 2.35                     | 0.62              |
| 46:Y0:27:GLU:HG3   | 46:Y0:68:GLU:HA    | 1.82                     | 0.62              |
| 50:Y4:37:SER:HB3   | 50:Y4:42:PHE:CD1   | 2.35                     | 0.62              |
| 54:Y8:23:VAL:HG11  | 54:Y8:46:ARG:HD3   | 1.81                     | 0.62              |
| 25:YA:1798:U:C5'   | 27:YD:259:THR:HG22 | 2.29                     | 0.62              |
| 25:RA:630:G:N2     | 25:RA:633:A:OP2    | 2.32                     | 0.61              |
| 1:XA:1500:A:H5''   | 1:XA:1508:G:H5''   | 1.81                     | 0.61              |
| 4:XD:111:ALA:HB2   | 4:XD:120:LEU:HD12  | 1.82                     | 0.61              |
| 5:XE:42:GLY:HA3    | 5:XE:66:MET:HG2    | 1.82                     | 0.61              |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:N    | 2.15                     | 0.61              |
| 27:YD:248:SER:HB3  | 27:YD:252:TRP:CE2  | 2.34                     | 0.61              |
| 40:YU:92:ARG:HD2   | 41:YV:11:GLN:HB2   | 1.82                     | 0.61              |
| 28:RE:67:PHE:O     | 28:RE:69:LYS:N     | 2.32                     | 0.61              |
| 32:RI:104:GLN:O    | 32:RI:105:HIS:ND1  | 2.33                     | 0.61              |
| 32:RI:57:ARG:HA    | 32:RI:60:GLU:HB3   | 1.81                     | 0.61              |
| 1:XA:560:U:O2'     | 1:XA:561:U:OP2     | 2.14                     | 0.61              |
| 29:YF:197:ASP:OD1  | 29:YF:197:ASP:N    | 2.33                     | 0.61              |
| 38:YS:83:LYS:C     | 38:YS:109:GLY:HA3  | 2.21                     | 0.61              |
| 12:QL:57:LYS:HG2   | 12:QL:67:THR:HG22  | 1.81                     | 0.61              |
| 25:RA:1272:A:OP2   | 25:RA:1647:G:OP1   | 2.18                     | 0.61              |
| 9:XI:29:ASN:OD1    | 9:XI:65:VAL:N      | 2.29                     | 0.61              |
| 25:YA:2030:A:H4'   | 25:YA:2031:A:C8    | 2.36                     | 0.61              |
| 1:QA:1077:G:N2     | 1:QA:1080:A:OP2    | 2.29                     | 0.61              |
| 10:QJ:40:LEU:HB2   | 10:QJ:69:ASN:HB3   | 1.82                     | 0.61              |
| 14:QN:13:THR:N     | 14:QN:14:PRO:HD2   | 2.15                     | 0.61              |
| 25:RA:2011:U:OP2   | 42:RW:16:LYS:NZ    | 2.30                     | 0.61              |
| 28:RE:51:PHE:CD2   | 28:RE:52:LEU:HG    | 2.34                     | 0.61              |
| 29:RF:28:ILE:HG22  | 29:RF:112:MET:HB3  | 1.80                     | 0.61              |
| 19:XS:5:LEU:HD21   | 50:Y4:66:SER:HB2   | 1.82                     | 0.61              |
| 1:QA:973:G:OP1     | 10:QJ:57:LYS:NZ    | 2.34                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:QC:14:ILE:O      | 3:QC:16:ARG:N      | 2.33                     | 0.61              |
| 4:QD:30:LYS:C      | 4:QD:32:ALA:N      | 2.52                     | 0.61              |
| 11:QK:22:HIS:HB3   | 11:QK:29:ILE:HG23  | 1.83                     | 0.61              |
| 1:QA:754:C:H5'     | 15:QO:72:ARG:HH22  | 1.65                     | 0.61              |
| 47:R1:53:VAL:HG22  | 47:R1:74:VAL:HG13  | 1.83                     | 0.61              |
| 55:R9:25:VAL:HB    | 55:R9:34:GLN:HB2   | 1.81                     | 0.61              |
| 25:RA:2405:G:O2'   | 25:RA:2411:A:N6    | 2.33                     | 0.61              |
| 25:RA:884:C:N3     | 25:RA:892:G:O6     | 2.33                     | 0.61              |
| 1:QA:1432:G:OP1    | 39:RT:107:ASP:HB2  | 2.00                     | 0.61              |
| 45:RZ:166:SER:HB2  | 45:RZ:168:GLU:H    | 1.64                     | 0.61              |
| 1:XA:745:C:OP1     | 1:XA:851:G:O2'     | 2.18                     | 0.61              |
| 2:XB:67:THR:HG21   | 2:XB:155:LEU:HG    | 1.81                     | 0.61              |
| 25:YA:2015:A:N3    | 51:Y5:2:ALA:N      | 2.48                     | 0.61              |
| 25:YA:392:C:H5''   | 25:YA:409:C:H5''   | 1.81                     | 0.61              |
| 4:QD:167:GLY:CA    | 27:YD:135:PHE:CZ   | 2.71                     | 0.61              |
| 1:QA:890:G:O2'     | 1:QA:906:G:O6      | 2.16                     | 0.61              |
| 1:QA:110:C:O2'     | 16:QP:25:ARG:O     | 2.17                     | 0.61              |
| 21:QU:6:ARG:HE     | 21:QU:15:ARG:NH2   | 1.99                     | 0.61              |
| 25:RA:997:G:OP1    | 40:RU:93:LYS:HD3   | 2.00                     | 0.61              |
| 19:XS:68:GLY:N     | 50:Y4:59:PHE:CZ    | 2.67                     | 0.61              |
| 25:RA:2444:G:OP2   | 29:RF:68:LYS:HE3   | 2.00                     | 0.61              |
| 32:RI:5:LEU:HD13   | 32:RI:17:GLN:HB3   | 1.81                     | 0.61              |
| 35:RP:84:ASN:HB3   | 35:RP:86:LYS:HG2   | 1.83                     | 0.61              |
| 36:RQ:65:PHE:O     | 36:RQ:67:ARG:N     | 2.34                     | 0.61              |
| 15:XO:87:ILE:HG22  | 15:XO:88:ARG:H     | 1.64                     | 0.61              |
| 25:YA:1045:A:C8    | 25:YA:1111:A:N6    | 2.68                     | 0.61              |
| 25:YA:2099:U:O4    | 25:YA:2190:G:O6    | 2.18                     | 0.61              |
| 36:YQ:134:ARG:NE   | 45:YZ:122:ARG:NH2  | 2.49                     | 0.61              |
| 2:QB:178:ARG:HH21  | 8:QH:74:PRO:HG3    | 1.66                     | 0.61              |
| 4:QD:105:VAL:HG13  | 4:QD:110:PHE:HB2   | 1.83                     | 0.61              |
| 15:QO:82:ILE:O     | 15:QO:86:GLY:N     | 2.33                     | 0.61              |
| 1:XA:949:A:N7      | 13:XM:106:ASN:ND2  | 2.48                     | 0.61              |
| 1:QA:1292:U:OP1    | 7:QG:41:ARG:NH2    | 2.33                     | 0.61              |
| 14:QN:6:LEU:HD23   | 14:QN:23:ARG:HH22  | 1.64                     | 0.61              |
| 42:RW:25:ARG:NH2   | 42:RW:74:ALA:O     | 2.33                     | 0.61              |
| 8:XH:4:ASP:OD2     | 8:XH:85:ARG:NH1    | 2.34                     | 0.61              |
| 47:Y1:83:GLU:O     | 47:Y1:85:LEU:N     | 2.34                     | 0.61              |
| 25:YA:573:G:N1     | 25:YA:2031:A:OP2   | 2.20                     | 0.61              |
| 31:YH:113:VAL:HG11 | 31:YH:151:ILE:HD12 | 1.83                     | 0.61              |
| 1:QA:501:C:H2'     | 1:QA:502:G:C8      | 2.35                     | 0.61              |
| 25:RA:1798:U:H5'   | 27:RD:259:THR:HG22 | 1.83                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:856:C:O2'   | 25:RA:857:C:OP1    | 2.16                     | 0.61              |
| 25:RA:468:G:H4'   | 29:RF:62:ARG:HH12  | 1.65                     | 0.61              |
| 31:RH:8:PRO:HG2   | 31:RH:69:ARG:HE    | 1.66                     | 0.61              |
| 25:YA:2864:G:OP1  | 39:YT:119:LYS:HD2  | 2.01                     | 0.61              |
| 27:YD:108:PRO:HB3 | 27:YD:143:HIS:CE1  | 2.35                     | 0.61              |
| 40:YU:52:ARG:HA   | 40:YU:55:ARG:HG3   | 1.83                     | 0.61              |
| 25:RA:2712:U:HO2' | 25:RA:2712(A):A:H8 | 1.47                     | 0.60              |
| 25:RA:910:A:C5    | 36:RQ:13:GLN:HG3   | 2.36                     | 0.60              |
| 37:RR:70:LEU:O    | 37:RR:72:ASP:N     | 2.31                     | 0.60              |
| 25:RA:994:C:OP2   | 40:RU:54:LYS:NZ    | 2.34                     | 0.60              |
| 1:XA:1414:U:H2'   | 1:XA:1415:G:H8     | 1.65                     | 0.60              |
| 1:XA:842:C:O2'    | 1:XA:848:C:N4      | 2.34                     | 0.60              |
| 25:YA:2692:C:O2   | 25:YA:2847:U:O2'   | 2.18                     | 0.60              |
| 27:YD:72:LYS:NZ   | 27:YD:99:ASP:OD2   | 2.33                     | 0.60              |
| 45:YZ:58:VAL:O    | 45:YZ:60:GLU:N     | 2.34                     | 0.60              |
| 13:QM:7:VAL:HB    | 30:RG:115:ARG:NH1  | 2.16                     | 0.60              |
| 39:RT:77:PRO:HB2  | 39:RT:80:SER:HB2   | 1.83                     | 0.60              |
| 40:RU:90:VAL:HG11 | 41:RV:40:LEU:HD12  | 1.82                     | 0.60              |
| 12:XL:50:SER:O    | 12:XL:51:ALA:CB    | 2.49                     | 0.60              |
| 52:Y6:25:LYS:HZ2  | 54:Y8:34:TRP:HZ2   | 1.47                     | 0.60              |
| 25:YA:774:A:H2    | 25:YA:787:U:HO2'   | 1.48                     | 0.60              |
| 36:YQ:35:VAL:HG13 | 36:YQ:130:LYS:HB3  | 1.83                     | 0.60              |
| 3:QC:11:ARG:O     | 3:QC:13:GLY:N      | 2.34                     | 0.60              |
| 3:QC:8:ILE:HG23   | 3:QC:16:ARG:HG2    | 1.83                     | 0.60              |
| 25:RA:1296:G:OP1  | 25:RA:2709:G:O2'   | 2.11                     | 0.60              |
| 25:RA:155:C:N4    | 25:RA:171:G:H1     | 1.99                     | 0.60              |
| 25:RA:873:G:H1    | 25:RA:904:C:N4     | 1.98                     | 0.60              |
| 27:RD:44:ASN:HB3  | 27:RD:49:ILE:HA    | 1.83                     | 0.60              |
| 1:XA:1299:A:H2'   | 1:XA:1301:U:H1'    | 1.82                     | 0.60              |
| 31:YH:150:ALA:O   | 31:YH:152:ARG:N    | 2.34                     | 0.60              |
| 25:YA:2469:A:O2'  | 36:YQ:56:ARG:HG2   | 2.01                     | 0.60              |
| 25:RA:1782:C:H1'  | 25:RA:2609:U:H5''  | 1.82                     | 0.60              |
| 25:RA:2443:C:H2'  | 25:RA:2444:G:H8    | 1.66                     | 0.60              |
| 1:XA:1510:U:H2'   | 1:XA:1511:G:C8     | 2.36                     | 0.60              |
| 1:XA:1308:U:OP2   | 13:XM:99:ARG:HD2   | 2.02                     | 0.60              |
| 17:XQ:11:VAL:HG12 | 17:XQ:85:VAL:HG13  | 1.83                     | 0.60              |
| 51:Y5:16:ARG:HH11 | 51:Y5:16:ARG:HG2   | 1.66                     | 0.60              |
| 25:YA:1203:G:H3'  | 25:YA:1204:A:H5''  | 1.83                     | 0.60              |
| 25:YA:1652:A:OP1  | 37:YR:8:ARG:NH1    | 2.33                     | 0.60              |
| 35:YP:95:VAL:HG13 | 35:YP:100:LEU:HD21 | 1.83                     | 0.60              |
| 23:QW:48:C:H2'    | 23:QW:59:U:H4'     | 1.83                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:R5:57:VAL:HG13 | 51:R5:57:VAL:O     | 2.01                     | 0.60              |
| 25:RA:993:G:OP1   | 40:RU:50:ARG:NH2   | 2.34                     | 0.60              |
| 27:RD:70:TRP:CH2  | 27:RD:150:LYS:HA   | 2.36                     | 0.60              |
| 25:RA:252:G:OP2   | 35:RP:50:ARG:NH1   | 2.33                     | 0.60              |
| 38:RS:88:ASP:O    | 38:RS:89:ARG:HB3   | 2.02                     | 0.60              |
| 1:XA:1243:C:H42   | 1:XA:1294:G:H1     | 1.49                     | 0.60              |
| 25:YA:2131:G:H4'  | 25:YA:2132:U:H4'   | 1.84                     | 0.60              |
| 27:YD:35:LYS:HD2  | 27:YD:104:TYR:CD1  | 2.35                     | 0.60              |
| 28:YE:9:VAL:HB    | 28:YE:25:VAL:HG23  | 1.83                     | 0.60              |
| 9:QI:13:ALA:HB2   | 9:QI:68:GLY:HA3    | 1.82                     | 0.60              |
| 1:XA:1266:G:N2    | 1:XA:1269:A:OP2    | 2.31                     | 0.60              |
| 1:XA:1314:C:OP1   | 19:XS:6:LYS:HE3    | 2.00                     | 0.60              |
| 25:YA:252:G:OP2   | 35:YP:50:ARG:NH1   | 2.35                     | 0.60              |
| 28:YE:25:VAL:HG12 | 28:YE:183:LEU:HG   | 1.84                     | 0.60              |
| 34:YO:96:THR:O    | 34:YO:97:ARG:HB3   | 2.01                     | 0.60              |
| 39:YT:84:GLN:OE1  | 39:YT:85:LYS:NZ    | 2.34                     | 0.60              |
| 1:QA:864:A:H5'    | 5:QE:86:ALA:HB2    | 1.83                     | 0.60              |
| 15:QO:39:LEU:HD13 | 15:QO:56:LEU:HB2   | 1.83                     | 0.60              |
| 50:R4:23:GLU:O    | 50:R4:25:TYR:N     | 2.33                     | 0.60              |
| 25:RA:1169:G:H1   | 25:RA:1180:C:H42   | 0.70                     | 0.60              |
| 54:Y8:50:LEU:HD12 | 54:Y8:51:ALA:H     | 1.67                     | 0.60              |
| 55:Y9:35:ARG:HH21 | 55:Y9:37:GLY:HA3   | 1.67                     | 0.60              |
| 25:YA:530:G:O2'   | 25:YA:532:A:N7     | 2.35                     | 0.60              |
| 30:YG:28:VAL:HG23 | 30:YG:29:TRP:CD1   | 2.36                     | 0.60              |
| 31:YH:152:ARG:CG  | 31:YH:153:LYS:HD2  | 2.28                     | 0.60              |
| 31:YH:4:ILE:HB    | 31:YH:6:ARG:HG2    | 1.82                     | 0.60              |
| 1:QA:1305:G:H22   | 1:QA:1331:G:H2'    | 1.66                     | 0.60              |
| 2:QB:15:VAL:H     | 2:QB:16:HIS:CE1    | 2.20                     | 0.60              |
| 1:QA:1106:G:H5''  | 3:QC:172:ARG:HG2   | 1.84                     | 0.60              |
| 1:XA:674:G:H2'    | 1:XA:675:A:C8      | 2.36                     | 0.60              |
| 13:XM:3:ARG:HA    | 13:XM:9:ILE:HG21   | 1.83                     | 0.60              |
| 23:XW:49:C:H42    | 23:XW:65:G:H1      | 1.47                     | 0.60              |
| 25:YA:2335:A:O2'  | 25:YA:2336:A:O5'   | 2.15                     | 0.60              |
| 25:YA:2377:A:H2'  | 25:YA:2378:A:C8    | 2.37                     | 0.60              |
| 32:YI:21:VAL:HG21 | 32:YI:25:TYR:HD2   | 1.66                     | 0.60              |
| 35:YP:147:LEU:O   | 35:YP:148:LEU:HB2  | 2.02                     | 0.60              |
| 45:YZ:54:HIS:O    | 45:YZ:98:MET:HE2   | 2.00                     | 0.60              |
| 12:QL:84:LEU:HD22 | 12:QL:104:VAL:HG11 | 1.84                     | 0.60              |
| 19:QS:67:VAL:CA   | 50:R4:59:PHE:CZ    | 2.85                     | 0.60              |
| 51:R5:16:ARG:HH11 | 51:R5:16:ARG:HG2   | 1.66                     | 0.60              |
| 44:RY:87:LYS:O    | 44:RY:88:LYS:NZ    | 2.33                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1002:G:H1     | 1:XA:1038:C:N4     | 1.98                     | 0.60              |
| 1:XA:826:C:H2'     | 1:XA:827:U:O2      | 2.01                     | 0.60              |
| 1:QA:344:A:O2'     | 1:QA:346:G:O6      | 2.18                     | 0.60              |
| 7:QG:149:ARG:NE    | 11:QK:59:TYR:CE1   | 2.70                     | 0.60              |
| 7:QG:26:PHE:O      | 7:QG:30:ILE:HG12   | 2.01                     | 0.60              |
| 9:QI:9:ARG:HB3     | 9:QI:14:VAL:HG13   | 1.84                     | 0.60              |
| 10:QJ:42:THR:HG23  | 10:QJ:68:HIS:HA    | 1.83                     | 0.60              |
| 25:RA:49:A:N7      | 25:RA:120:U:O4     | 2.33                     | 0.60              |
| 26:RB:31:C:H42     | 26:RB:51:G:H1      | 1.50                     | 0.60              |
| 30:RG:114:ILE:HD13 | 30:RG:140:ILE:HG21 | 1.83                     | 0.60              |
| 31:RH:154:PRO:HD3  | 31:RH:162:ILE:N    | 2.16                     | 0.60              |
| 4:QD:194:LEU:HD11  | 6:XF:17:SER:OG     | 2.02                     | 0.60              |
| 25:YA:137(A):G:H1' | 43:YX:41:ASN:ND2   | 2.16                     | 0.60              |
| 1:QA:1446:A:H4'    | 39:RT:125:ARG:HH22 | 1.67                     | 0.59              |
| 39:RT:105:LEU:O    | 39:RT:107:ASP:N    | 2.35                     | 0.59              |
| 45:RZ:144:LEU:HG   | 45:RZ:150:LEU:HD12 | 1.84                     | 0.59              |
| 28:YE:14:ILE:HG22  | 28:YE:21:VAL:HG23  | 0.69                     | 0.59              |
| 37:YR:42:LYS:HA    | 37:YR:45:ARG:HD2   | 1.84                     | 0.59              |
| 31:RH:89:ILE:HD13  | 31:RH:129:THR:HB   | 1.83                     | 0.59              |
| 2:XB:235:SER:O     | 2:XB:237:ALA:N     | 2.36                     | 0.59              |
| 54:R8:29:LYS:HB2   | 54:R8:44:LYS:HG2   | 1.84                     | 0.59              |
| 30:RG:64:THR:HG23  | 30:RG:66:GLN:H     | 1.66                     | 0.59              |
| 38:RS:38:GLN:OE1   | 38:RS:47:THR:OG1   | 2.18                     | 0.59              |
| 1:XA:380:G:N2      | 1:XA:383:A:OP2     | 2.32                     | 0.59              |
| 2:XB:92:TYR:HE1    | 2:XB:151:GLY:HA3   | 1.65                     | 0.59              |
| 4:QD:195:ALA:CB    | 6:XF:20:ALA:CB     | 2.81                     | 0.59              |
| 25:YA:2298:A:H62   | 25:YA:2318:G:H8    | 1.50                     | 0.59              |
| 26:YB:40:U:O2'     | 26:YB:45:A:N6      | 2.32                     | 0.59              |
| 31:YH:98:LEU:HD22  | 31:YH:125:VAL:HB   | 1.83                     | 0.59              |
| 32:YI:129:THR:HG22 | 32:YI:137:PRO:HB3  | 1.84                     | 0.59              |
| 42:YW:86:LEU:HD12  | 42:YW:87:PRO:HD2   | 1.83                     | 0.59              |
| 42:YW:90:ARG:CG    | 42:YW:90:ARG:HH11  | 2.14                     | 0.59              |
| 1:QA:1061:G:OP1    | 10:QJ:59:SER:OG    | 2.21                     | 0.59              |
| 45:RZ:52:SER:O     | 45:RZ:52:SER:OG    | 2.12                     | 0.59              |
| 45:RZ:87:ASP:N     | 45:RZ:87:ASP:OD1   | 2.34                     | 0.59              |
| 1:XA:1432:G:OP1    | 39:YT:107:ASP:HB2  | 2.03                     | 0.59              |
| 1:XA:1450:U:O2'    | 1:XA:1451:A:N7     | 2.34                     | 0.59              |
| 1:XA:570:G:O6      | 1:XA:865:A:N6      | 2.36                     | 0.59              |
| 26:YB:44:G:H1'     | 26:YB:47:C:H42     | 1.67                     | 0.59              |
| 35:YP:62:LEU:HB2   | 54:Y8:30:ARG:NH1   | 2.17                     | 0.59              |
| 37:YR:33:ARG:NH2   | 51:Y5:55:ARG:HG2   | 2.17                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:1352:C:OP1    | 21:QU:3:LYS:NZ    | 2.29                     | 0.59              |
| 25:RA:1291:C:H5'   | 25:RA:1536:A:H5'  | 1.85                     | 0.59              |
| 30:RG:67:LYS:HE2   | 50:R4:6:HIS:CE1   | 2.38                     | 0.59              |
| 49:Y3:6:VAL:HG13   | 49:Y3:56:VAL:HG13 | 1.84                     | 0.59              |
| 53:Y7:35:ARG:HG3   | 53:Y7:42:LEU:HD11 | 1.85                     | 0.59              |
| 28:YE:36:ARG:HH21  | 28:YE:88:GLY:HA2  | 1.68                     | 0.59              |
| 1:QA:1172:C:H2'    | 1:QA:1173:G:C8    | 2.38                     | 0.59              |
| 3:QC:50:ALA:HB2    | 3:QC:75:VAL:HB    | 1.85                     | 0.59              |
| 25:RA:1026:U:H4'   | 25:RA:1027:A:OP1  | 2.02                     | 0.59              |
| 25:RA:83:G:N2      | 25:RA:103:A:OP2   | 2.31                     | 0.59              |
| 13:QM:8:GLU:OE1    | 30:RG:115:ARG:NE  | 2.35                     | 0.59              |
| 42:RW:86:LEU:HD12  | 42:RW:87:PRO:HD2  | 1.85                     | 0.59              |
| 25:YA:2126:A:H4'   | 25:YA:2127:G:O5'  | 2.03                     | 0.59              |
| 25:YA:49:A:N7      | 25:YA:120:U:C5    | 2.70                     | 0.59              |
| 25:YA:855:G:H1     | 25:YA:922:U:H3    | 1.51                     | 0.59              |
| 13:QM:49:THR:HB    | 13:QM:52:GLU:HG3  | 1.85                     | 0.59              |
| 25:RA:577:G:O2'    | 25:RA:1254:A:OP1  | 2.18                     | 0.59              |
| 28:RE:21:VAL:HB    | 28:RE:22:PRO:HA   | 1.85                     | 0.59              |
| 1:XA:1178:G:N2     | 1:XA:1181:G:N7    | 2.49                     | 0.59              |
| 1:XA:67:C:H2'      | 1:XA:68:G:C8      | 2.38                     | 0.59              |
| 13:XM:121:LYS:NZ   | 23:XY:40:C:O3'    | 2.35                     | 0.59              |
| 25:YA:27:G:H1'     | 25:YA:513:A:N6    | 2.17                     | 0.59              |
| 42:YW:111:HIS:CD2  | 42:YW:112:GLY:H   | 2.20                     | 0.59              |
| 56:Z8:1:T17:H66    | 56:Z8:2:GLY:N     | 2.17                     | 0.59              |
| 1:QA:1023:G:H3'    | 1:QA:1024:G:H5''  | 1.83                     | 0.59              |
| 52:R6:52:VAL:HG22  | 52:R6:53:LYS:HG3  | 1.84                     | 0.59              |
| 25:RA:630:G:OP1    | 54:R8:46:ARG:NH1  | 2.35                     | 0.59              |
| 31:RH:121:ILE:HG13 | 31:RH:140:LYS:HD2 | 1.84                     | 0.59              |
| 1:XA:427:U:OP1     | 4:XD:13:ARG:NH2   | 2.35                     | 0.59              |
| 6:XF:61:LEU:HB3    | 6:XF:63:TYR:HE1   | 1.66                     | 0.59              |
| 1:XA:690:G:H22     | 11:XK:55:LYS:NZ   | 2.01                     | 0.59              |
| 20:XT:10:LEU:HG    | 20:XT:12:ALA:H    | 1.67                     | 0.59              |
| 25:YA:330:A:HO2'   | 25:YA:331:A:H8    | 1.51                     | 0.59              |
| 32:YI:67:ARG:HH21  | 32:YI:68:LEU:HB2  | 1.68                     | 0.59              |
| 35:YP:26:GLY:O     | 35:YP:28:GLY:N    | 2.35                     | 0.59              |
| 4:QD:166:LYS:HG3   | 4:QD:178:VAL:CG1  | 2.20                     | 0.59              |
| 7:QG:73:MET:HG2    | 7:QG:90:GLU:HA    | 1.83                     | 0.59              |
| 16:QP:21:VAL:O     | 16:QP:33:ILE:HG12 | 2.02                     | 0.59              |
| 19:QS:64:GLU:CD    | 50:R4:55:ARG:HH12 | 2.06                     | 0.59              |
| 25:RA:1359:A:N6    | 25:RA:1372:U:C5   | 2.70                     | 0.59              |
| 25:RA:1636:C:H2'   | 25:RA:1637:A:C8   | 2.38                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2010:G:H5''  | 42:RW:42:ARG:HB2   | 1.85                     | 0.59              |
| 26:RB:50:G:H5''    | 38:RS:61:ASN:HD21  | 1.67                     | 0.59              |
| 31:RH:105:LEU:HD13 | 31:RH:105:LEU:H    | 1.68                     | 0.59              |
| 36:RQ:109:VAL:HG12 | 36:RQ:114:ALA:HB2  | 1.84                     | 0.59              |
| 1:XA:1128:C:H5'    | 9:XI:16:ARG:HH22   | 1.67                     | 0.59              |
| 10:XJ:76:ASN:O     | 10:XJ:78:ASN:ND2   | 2.36                     | 0.59              |
| 23:XW:11:C:H42     | 23:XW:24:G:H1      | 1.49                     | 0.59              |
| 26:YB:44:G:OP1     | 50:Y4:1:MET:N      | 2.36                     | 0.59              |
| 31:YH:6:ARG:NH2    | 31:YH:54:ARG:HH22  | 2.01                     | 0.59              |
| 4:QD:64:LEU:HB2    | 4:QD:198:VAL:HG11  | 1.83                     | 0.59              |
| 7:QG:149:ARG:HD3   | 11:QK:59:TYR:CZ    | 2.38                     | 0.59              |
| 19:QS:68:GLY:HA3   | 50:R4:69:LYS:H     | 1.66                     | 0.59              |
| 47:R1:92:LYS:HG3   | 47:R1:96:LYS:HB2   | 1.84                     | 0.59              |
| 50:R4:16:CYS:SG    | 50:R4:17:GLY:N     | 2.75                     | 0.59              |
| 27:RD:85:ASP:HB2   | 27:RD:92:ILE:HD13  | 1.84                     | 0.59              |
| 5:XE:45:PHE:CE2    | 5:XE:47:LYS:HD2    | 2.38                     | 0.59              |
| 25:YA:2636:U:OP1   | 28:YE:79:ARG:HA    | 2.03                     | 0.59              |
| 25:YA:2646:C:OP2   | 25:YA:2732:G:O2'   | 2.15                     | 0.59              |
| 38:YS:26:LEU:HB3   | 38:YS:87:PHE:HA    | 1.85                     | 0.59              |
| 1:QA:56:U:H2'      | 1:QA:57:G:C8       | 2.38                     | 0.58              |
| 25:RA:617:G:OP1    | 29:RF:40:GLN:NE2   | 2.26                     | 0.58              |
| 1:XA:1443:G:H5''   | 1:XA:1446:A:H2     | 1.67                     | 0.58              |
| 3:XC:14:ILE:HG12   | 3:XC:15:THR:H      | 1.67                     | 0.58              |
| 12:XL:38:THR:HG23  | 12:XL:57:LYS:HB3   | 1.84                     | 0.58              |
| 14:XN:23:ARG:HD2   | 14:XN:28:GLY:O     | 2.03                     | 0.58              |
| 27:YD:28:GLU:OE1   | 27:YD:29:PRO:HD2   | 2.03                     | 0.58              |
| 30:YG:136:ARG:O    | 30:YG:154:GLY:HA2  | 2.02                     | 0.58              |
| 31:YH:15:VAL:HG12  | 31:YH:28:GLY:HA3   | 1.83                     | 0.58              |
| 1:QA:359:U:P       | 32:YI:87:LYS:HE2   | 2.42                     | 0.58              |
| 33:YN:40:PRO:HB3   | 40:YU:68:ALA:HB2   | 1.85                     | 0.58              |
| 8:QH:121:ASP:N     | 8:QH:121:ASP:OD1   | 2.34                     | 0.58              |
| 25:RA:1918:A:O2'   | 25:RA:1920:C:N4    | 2.36                     | 0.58              |
| 25:RA:259:G:H21    | 25:RA:621:A:H8     | 1.51                     | 0.58              |
| 27:RD:71:ASP:OD2   | 27:RD:103:ARG:NH2  | 2.36                     | 0.58              |
| 30:RG:112:PRO:HB3  | 50:R4:37:SER:HB2   | 1.85                     | 0.58              |
| 45:RZ:158:PRO:HG2  | 45:RZ:161:VAL:HG21 | 1.85                     | 0.58              |
| 4:XD:20:TYR:HA     | 4:XD:26:CYS:SG     | 2.43                     | 0.58              |
| 25:YA:2581:G:OP2   | 25:YA:2581:G:N2    | 2.36                     | 0.58              |
| 37:YR:67:LEU:HD13  | 37:YR:76:VAL:HG21  | 1.84                     | 0.58              |
| 38:YS:106:ARG:HA   | 38:YS:110:LEU:HD11 | 1.86                     | 0.58              |
| 43:YX:61:GLY:N     | 43:YX:75:ASP:OD1   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:119:A:H4'    | 1:QA:120:A:O5'    | 2.02                     | 0.58              |
| 4:QD:111:ALA:HB2  | 4:QD:120:LEU:HD12 | 1.85                     | 0.58              |
| 25:RA:102:G:H4'   | 25:RA:103:A:O5'   | 2.03                     | 0.58              |
| 27:RD:44:ASN:CB   | 27:RD:49:ILE:HA   | 2.33                     | 0.58              |
| 32:RI:55:ALA:HA   | 32:RI:58:LEU:CB   | 2.32                     | 0.58              |
| 12:XL:47:LYS:HB3  | 12:XL:48:PRO:CD   | 2.33                     | 0.58              |
| 35:YP:58:THR:HG22 | 35:YP:61:ARG:HG3  | 1.85                     | 0.58              |
| 41:YV:44:LYS:O    | 41:YV:46:VAL:N    | 2.36                     | 0.58              |
| 10:QJ:49:VAL:HG13 | 14:QN:41:ARG:HB2  | 1.86                     | 0.58              |
| 25:RA:1309:G:H4'  | 53:R7:7:PRO:HB2   | 1.85                     | 0.58              |
| 28:RE:13:ARG:HH11 | 28:RE:21:VAL:HG11 | 1.68                     | 0.58              |
| 32:RI:110:ASP:N   | 32:RI:130:TYR:OH  | 2.30                     | 0.58              |
| 45:RZ:110:GLY:HA2 | 45:RZ:112:ARG:HB2 | 1.84                     | 0.58              |
| 1:XA:890:G:O2'    | 1:XA:906:G:O6     | 2.19                     | 0.58              |
| 2:XB:72:GLY:HA2   | 2:XB:165:VAL:HG22 | 1.85                     | 0.58              |
| 13:XM:13:LYS:HA   | 13:XM:44:ARG:HD2  | 1.83                     | 0.58              |
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21 | 1.84                     | 0.58              |
| 1:QA:352:C:O2'    | 1:QA:354:G:OP1    | 2.16                     | 0.58              |
| 25:RA:1226:G:H4'  | 41:RV:84:LYS:HG2  | 1.84                     | 0.58              |
| 25:RA:1579:A:H2'  | 25:RA:1580:A:C8   | 2.38                     | 0.58              |
| 25:RA:1899:G:H21  | 25:RA:1902:C:N4   | 2.01                     | 0.58              |
| 25:RA:2680:C:H5'  | 28:RE:189:PRO:HA  | 1.84                     | 0.58              |
| 27:RD:182:LEU:N   | 27:RD:272:ALA:HB3 | 2.17                     | 0.58              |
| 1:XA:1129:C:H4'   | 1:XA:1130:A:H5'   | 1.84                     | 0.58              |
| 6:XF:36:ARG:NH1   | 6:XF:38:GLU:OE2   | 2.37                     | 0.58              |
| 9:XI:43:ALA:HA    | 9:XI:74:ILE:HD13  | 1.85                     | 0.58              |
| 20:XT:63:ILE:HG22 | 20:XT:77:ALA:HB1  | 1.86                     | 0.58              |
| 50:Y4:42:PHE:O    | 50:Y4:44:THR:N    | 2.36                     | 0.58              |
| 51:Y5:4:HIS:HB3   | 51:Y5:5:PRO:CD    | 2.33                     | 0.58              |
| 25:YA:1664:A:H61  | 25:YA:1996:C:N4   | 1.98                     | 0.58              |
| 25:YA:2292:C:P    | 38:YS:17:ARG:HH22 | 2.26                     | 0.58              |
| 1:QA:1201:A:HO2'  | 1:QA:1202:G:P     | 2.27                     | 0.58              |
| 4:QD:29:PRO:HD2   | 4:QD:30:LYS:HD3   | 1.84                     | 0.58              |
| 12:QL:53:ARG:HD3  | 12:QL:93:LEU:HD21 | 1.86                     | 0.58              |
| 13:QM:80:ARG:NE   | 50:R4:71:ARG:NH1  | 2.48                     | 0.58              |
| 30:RG:136:ARG:O   | 30:RG:154:GLY:HA2 | 2.03                     | 0.58              |
| 31:RH:89:ILE:O    | 31:RH:89:ILE:HG12 | 2.04                     | 0.58              |
| 1:XA:266:G:O2'    | 1:XA:267:C:OP2    | 2.16                     | 0.58              |
| 4:XD:22:LYS:HD2   | 4:XD:26:CYS:SG    | 2.44                     | 0.58              |
| 26:YB:15:A:H5'    | 26:YB:16:G:C8     | 2.39                     | 0.58              |
| 29:YF:127:GLU:O   | 29:YF:129:PHE:N   | 2.32                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:5:LEU:HD11   | 45:YZ:39:VAL:HB    | 1.85                     | 0.58              |
| 2:QB:77:ALA:HB2    | 2:QB:211:ILE:HD13  | 1.86                     | 0.58              |
| 36:RQ:78:PRO:O     | 46:R0:5:LYS:HE2    | 2.03                     | 0.58              |
| 25:RA:2611:U:O2    | 51:R5:3:LYS:HE3    | 2.02                     | 0.58              |
| 25:RA:2126:A:H4'   | 25:RA:2127:G:O5'   | 2.04                     | 0.58              |
| 27:RD:35:LYS:HD2   | 27:RD:104:TYR:CE1  | 2.39                     | 0.58              |
| 31:RH:87:LEU:HD22  | 31:RH:162:ILE:HG22 | 1.85                     | 0.58              |
| 1:XA:243:A:H4'     | 1:XA:244:U:O5'     | 2.03                     | 0.58              |
| 1:XA:753:A:H4'     | 1:XA:754:C:O5'     | 2.03                     | 0.58              |
| 2:XB:15:VAL:H      | 2:XB:16:HIS:CE1    | 2.22                     | 0.58              |
| 2:XB:96:ARG:H      | 2:XB:96:ARG:HD2    | 1.68                     | 0.58              |
| 8:XH:39:LEU:HB3    | 8:XH:45:ILE:HG12   | 1.86                     | 0.58              |
| 45:YZ:146:ILE:HG22 | 45:YZ:176:PRO:HD3  | 1.84                     | 0.58              |
| 1:QA:427:U:OP1     | 4:QD:13:ARG:NH2    | 2.36                     | 0.58              |
| 1:QA:1495:U:O2'    | 25:RA:1919:A:N1    | 2.32                     | 0.58              |
| 25:RA:654(A):G:H1  | 25:RA:654(T):C:H42 | 1.49                     | 0.58              |
| 27:RD:24:ILE:HD11  | 27:RD:91:ARG:HD2   | 1.84                     | 0.58              |
| 32:RI:5:LEU:H      | 32:RI:5:LEU:HD12   | 1.69                     | 0.58              |
| 2:XB:93:VAL:HG11   | 2:XB:97:TRP:HD1    | 1.68                     | 0.58              |
| 3:XC:95:THR:HG22   | 3:XC:97:LYS:HG3    | 1.83                     | 0.58              |
| 20:XT:56:MET:HG3   | 20:XT:88:VAL:HG21  | 1.86                     | 0.58              |
| 34:YO:64:ARG:HG2   | 34:YO:79:PHE:CG    | 2.38                     | 0.58              |
| 1:QA:382:A:H2'     | 1:QA:383:A:C8      | 2.39                     | 0.58              |
| 25:RA:1266:G:O5'   | 42:RW:15:ARG:NH2   | 2.37                     | 0.58              |
| 35:RP:47:ASP:OD2   | 35:RP:49:ARG:NH1   | 2.37                     | 0.58              |
| 19:XS:5:LEU:CD2    | 50:Y4:66:SER:HB2   | 2.33                     | 0.58              |
| 25:YA:1068:G:O2'   | 25:YA:1096:A:N3    | 2.37                     | 0.58              |
| 1:QA:181:G:O2'     | 1:QA:182:U:O5'     | 2.20                     | 0.58              |
| 14:QN:24:CYS:HB3   | 14:QN:27:CYS:SG    | 2.40                     | 0.58              |
| 33:RN:54:VAL:HB    | 33:RN:122:VAL:HG22 | 1.85                     | 0.58              |
| 1:XA:1108:G:H5'    | 3:XC:176:HIS:ND1   | 2.18                     | 0.58              |
| 1:XA:686:U:HO2'    | 11:XK:42:TRP:HE1   | 1.51                     | 0.58              |
| 17:XQ:55:ASP:HA    | 17:XQ:79:SER:HA    | 1.85                     | 0.58              |
| 32:YI:56:LYS:HE3   | 32:YI:57:ARG:HA    | 1.84                     | 0.58              |
| 37:YR:27:SER:HB3   | 37:YR:34:ILE:HD11  | 1.84                     | 0.58              |
| 1:QA:927:G:H1      | 1:QA:1390:U:H3     | 1.52                     | 0.57              |
| 13:QM:58:GLU:O     | 13:QM:62:ASN:ND2   | 2.31                     | 0.57              |
| 26:RB:44:G:OP1     | 50:R4:1:MET:N      | 2.35                     | 0.57              |
| 25:RA:414:C:O2     | 25:RA:1864:U:O2'   | 2.21                     | 0.57              |
| 25:RA:65:C:O2'     | 25:RA:456:C:N3     | 2.33                     | 0.57              |
| 28:RE:131:ALA:HB1  | 28:RE:135:HIS:HE1  | 1.69                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:RN:13:TRP:O     | 33:RN:135:PRO:HD2  | 2.03                     | 0.57              |
| 44:RY:95:LYS:NZ    | 44:RY:99:CYS:O     | 2.37                     | 0.57              |
| 36:RQ:135:ASP:OD2  | 45:RZ:81:ARG:NH1   | 2.37                     | 0.57              |
| 1:XA:1280:A:H1'    | 10:XJ:41:PRO:HG3   | 1.86                     | 0.57              |
| 5:XE:91:LEU:HD12   | 5:XE:120:THR:HG22  | 1.85                     | 0.57              |
| 1:XA:673:G:H5''    | 6:XF:87:ARG:NH1    | 2.19                     | 0.57              |
| 19:XS:39:THR:HG21  | 50:Y4:68:ARG:HG2   | 1.84                     | 0.57              |
| 19:XS:80:TYR:O     | 19:XS:82:GLY:N     | 2.36                     | 0.57              |
| 30:YG:98:ARG:NH1   | 50:Y4:1:MET:SD     | 2.77                     | 0.57              |
| 30:YG:67:LYS:HE2   | 50:Y4:6:HIS:CE1    | 2.38                     | 0.57              |
| 25:YA:125:G:H5''   | 53:Y7:19:ARG:HD3   | 1.86                     | 0.57              |
| 25:YA:221:A:H4'    | 25:YA:222:A:O5'    | 2.04                     | 0.57              |
| 29:YF:28:ILE:HG22  | 29:YF:112:MET:HB3  | 1.85                     | 0.57              |
| 37:YR:117:VAL:HG22 | 37:YR:118:GLU:H    | 1.68                     | 0.57              |
| 39:YT:24:PRO:HA    | 39:YT:49:VAL:HG13  | 1.85                     | 0.57              |
| 1:QA:559:A:H4'     | 1:QA:560:U:H3'     | 1.85                     | 0.57              |
| 3:QC:134:ILE:HG23  | 3:QC:151:VAL:HB    | 1.85                     | 0.57              |
| 7:QG:26:PHE:CE2    | 7:QG:30:ILE:HD11   | 2.38                     | 0.57              |
| 30:RG:68:PRO:HB2   | 30:RG:90:LEU:HD12  | 1.86                     | 0.57              |
| 42:RW:71:VAL:HA    | 42:RW:107:LEU:HD12 | 1.86                     | 0.57              |
| 1:XA:1077:G:N2     | 1:XA:1080:A:OP2    | 2.34                     | 0.57              |
| 3:XC:70:VAL:HG21   | 3:XC:76:VAL:HG11   | 1.85                     | 0.57              |
| 25:YA:1403:C:H5''  | 25:YA:1471:A:H1'   | 1.85                     | 0.57              |
| 25:YA:630:G:OP2    | 54:Y8:15:LYS:NZ    | 2.37                     | 0.57              |
| 28:YE:35:GLN:HB3   | 28:YE:48:GLN:HB2   | 1.86                     | 0.57              |
| 13:XM:68:GLY:HA3   | 30:YG:116:ASP:CG   | 2.25                     | 0.57              |
| 37:YR:24:GLN:OE1   | 37:YR:36:THR:HG21  | 2.04                     | 0.57              |
| 38:YS:10:ARG:NH2   | 38:YS:91:PRO:O     | 2.36                     | 0.57              |
| 42:YW:73:ALA:HB3   | 42:YW:106:ILE:HD13 | 1.84                     | 0.57              |
| 1:QA:1002:G:N2     | 1:QA:1038:C:N3     | 2.46                     | 0.57              |
| 25:RA:1490:A:O2'   | 27:RD:99:ASP:OD1   | 2.21                     | 0.57              |
| 1:XA:1453:G:H8     | 20:XT:39:LYS:HE2   | 1.69                     | 0.57              |
| 46:Y0:50:ASN:HB3   | 46:Y0:63:VAL:HG22  | 1.86                     | 0.57              |
| 25:YA:1899:G:H21   | 25:YA:1902:C:H41   | 1.51                     | 0.57              |
| 40:YU:92:ARG:HD3   | 40:YU:94:ASN:HB3   | 1.85                     | 0.57              |
| 1:QA:953:G:N7      | 13:QM:104:ARG:NH2  | 2.52                     | 0.57              |
| 3:QC:134:ILE:HG22  | 3:QC:168:ALA:HB3   | 1.86                     | 0.57              |
| 7:QG:79:ARG:HH12   | 7:QG:82:GLY:HA2    | 1.69                     | 0.57              |
| 46:R0:18:ALA:O     | 46:R0:20:ARG:NH1   | 2.36                     | 0.57              |
| 36:RQ:81:VAL:HG23  | 46:R0:7:LEU:CD1    | 2.34                     | 0.57              |
| 31:RH:153:LYS:HB3  | 31:RH:154:PRO:CD   | 2.34                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:559:A:OP1     | 5:XE:126:ARG:NH2   | 2.36                     | 0.57              |
| 11:XK:21:ILE:HG13  | 11:XK:30:VAL:HG12  | 1.86                     | 0.57              |
| 1:XA:686:U:H1'     | 11:XK:42:TRP:HE1   | 1.68                     | 0.57              |
| 11:XK:54:ARG:NH2   | 23:XW:39:U:O2'     | 2.38                     | 0.57              |
| 25:YA:247:G:H4'    | 25:YA:386:G:C5     | 2.39                     | 0.57              |
| 36:YQ:116:GLU:O    | 36:YQ:120:ILE:HG12 | 2.05                     | 0.57              |
| 1:QA:564:C:P       | 12:QL:15:ARG:HH21  | 2.26                     | 0.57              |
| 5:QE:143:ARG:HH21  | 8:QH:77:GLU:CD     | 2.07                     | 0.57              |
| 13:QM:14:ARG:N     | 13:QM:44:ARG:HD3   | 2.17                     | 0.57              |
| 25:RA:330:A:H2     | 25:RA:1210:A:H2'   | 1.70                     | 0.57              |
| 1:XA:538:G:H5''    | 12:XL:114:LYS:HB2  | 1.87                     | 0.57              |
| 4:XD:154:ASN:OD1   | 4:XD:154:ASN:N     | 2.37                     | 0.57              |
| 22:XV:0:C:O2'      | 46:Y0:6:GLY:O      | 2.21                     | 0.57              |
| 25:YA:1428:C:N4    | 25:YA:1570:A:OP2   | 2.36                     | 0.57              |
| 25:YA:2133:G:H1'   | 25:YA:2158:A:H61   | 1.70                     | 0.57              |
| 35:YP:135:LEU:O    | 35:YP:139:LYS:HB2  | 2.04                     | 0.57              |
| 36:YQ:66:ILE:HA    | 36:YQ:104:PHE:HA   | 1.85                     | 0.57              |
| 1:QA:1376:U:P      | 7:QG:94:ARG:HH12   | 2.28                     | 0.57              |
| 19:QS:67:VAL:HB    | 50:R4:59:PHE:CD2   | 2.38                     | 0.57              |
| 25:RA:307:G:N2     | 25:RA:309:G:H3'    | 2.20                     | 0.57              |
| 27:RD:145:VAL:HG13 | 27:RD:191:ALA:HB2  | 1.87                     | 0.57              |
| 37:RR:117:VAL:O    | 37:RR:118:GLU:HB2  | 2.05                     | 0.57              |
| 44:RY:76:CYS:SG    | 44:RY:77:PRO:HD2   | 2.45                     | 0.57              |
| 1:XA:1349:A:OP2    | 9:XI:118:LYS:NZ    | 2.29                     | 0.57              |
| 1:XA:74:C:H42      | 1:XA:96:G:H1       | 1.51                     | 0.57              |
| 4:XD:9:CYS:HB3     | 4:XD:32:ALA:HB2    | 1.87                     | 0.57              |
| 19:XS:32:LYS:HA    | 19:XS:50:ALA:HB3   | 1.86                     | 0.57              |
| 27:YD:65:ILE:H     | 27:YD:65:ILE:HD13  | 1.68                     | 0.57              |
| 28:YE:11:MET:HG2   | 28:YE:24:THR:OG1   | 2.04                     | 0.57              |
| 25:YA:138:G:N2     | 43:YX:44:GLU:OE2   | 2.29                     | 0.57              |
| 45:YZ:91:LEU:HG    | 45:YZ:130:PRO:CB   | 2.26                     | 0.57              |
| 25:RA:2442:C:OP1   | 56:Z7:6:LYS:NZ     | 2.38                     | 0.57              |
| 7:QG:15:ASP:OD1    | 7:QG:44:TYR:OH     | 2.22                     | 0.57              |
| 12:QL:10:LEU:HB3   | 17:QQ:32:TYR:CE2   | 2.40                     | 0.57              |
| 54:R8:36:LYS:HB3   | 54:R8:40:GLU:HG2   | 1.85                     | 0.57              |
| 25:RA:1378:A:OP1   | 53:R7:10:ARG:NH2   | 2.37                     | 0.57              |
| 2:XB:96:ARG:HD3    | 2:XB:148:TYR:HE1   | 1.70                     | 0.57              |
| 30:YG:98:ARG:HH12  | 50:Y4:1:MET:HB3    | 1.69                     | 0.57              |
| 31:YH:149:ARG:HG3  | 31:YH:162:ILE:O    | 2.05                     | 0.57              |
| 38:YS:52:SER:O     | 38:YS:55:ALA:O     | 2.21                     | 0.57              |
| 1:QA:1163:C:N4     | 1:QA:1173:G:H1     | 2.02                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:816:A:OP1     | 1:QA:1526:G:O2'    | 2.20                     | 0.57              |
| 25:RA:137(A):G:H1' | 43:RX:41:ASN:ND2   | 2.19                     | 0.57              |
| 25:RA:1045:A:C4    | 25:RA:1111:A:N6    | 2.73                     | 0.57              |
| 25:RA:1341:U:OP2   | 25:RA:1394:U:O2'   | 2.19                     | 0.57              |
| 25:RA:1936:A:OP2   | 25:RA:1962:C:N4    | 2.37                     | 0.57              |
| 25:RA:2735:G:H2'   | 25:RA:2736:G:H8    | 1.67                     | 0.57              |
| 27:RD:241:PRO:O    | 27:RD:242:ARG:HB2  | 2.04                     | 0.57              |
| 30:RG:22:ARG:HH21  | 30:RG:171:ALA:HB1  | 1.69                     | 0.57              |
| 35:RP:58:THR:C     | 35:RP:61:ARG:HE    | 2.06                     | 0.57              |
| 1:XA:437:U:H2'     | 1:XA:438:G:O4'     | 2.04                     | 0.57              |
| 16:XP:20:VAL:HG23  | 16:XP:35:LYS:HA    | 1.86                     | 0.57              |
| 25:YA:1534:G:N2    | 25:YA:1537:C:O2    | 2.38                     | 0.57              |
| 27:YD:71:ASP:CB    | 27:YD:103:ARG:HH22 | 2.18                     | 0.57              |
| 1:QA:1286:A:H5''   | 21:QU:26:LYS:HD2   | 1.85                     | 0.57              |
| 1:QA:765:G:N2      | 1:QA:813:U:OP2     | 2.38                     | 0.57              |
| 2:QB:51:LEU:HD23   | 2:QB:201:ILE:HD12  | 1.86                     | 0.57              |
| 6:QF:3:ARG:NH1     | 6:QF:38:GLU:OE2    | 2.37                     | 0.57              |
| 13:QM:23:TYR:HB3   | 13:QM:67:GLU:HG2   | 1.87                     | 0.57              |
| 19:QS:67:VAL:CB    | 50:R4:59:PHE:CE1   | 2.88                     | 0.57              |
| 25:RA:247:G:H4'    | 25:RA:386:G:C5     | 2.40                     | 0.57              |
| 27:RD:44:ASN:HB2   | 27:RD:48:ARG:O     | 2.05                     | 0.57              |
| 39:RT:41:ARG:HB2   | 39:RT:41:ARG:CZ    | 2.34                     | 0.57              |
| 1:XA:1126:U:H5     | 1:XA:1127:G:C4     | 2.22                     | 0.57              |
| 25:YA:857:C:OP2    | 46:Y0:77:ARG:NH2   | 2.37                     | 0.57              |
| 25:YA:1094:U:O2'   | 25:YA:1096:A:OP1   | 2.19                     | 0.57              |
| 34:YO:85:VAL:HG11  | 34:YO:114:ILE:HD11 | 1.87                     | 0.57              |
| 1:QA:973:G:O6      | 1:QA:974:A:N6      | 2.38                     | 0.56              |
| 25:RA:2335:A:O2'   | 25:RA:2336:A:O5'   | 2.23                     | 0.56              |
| 13:QM:3:ARG:NH2    | 30:RG:113:ARG:HH21 | 2.03                     | 0.56              |
| 41:RV:52:VAL:HG21  | 41:RV:55:ALA:HB3   | 1.87                     | 0.56              |
| 1:XA:1002:G:H2'    | 1:XA:1003:G:C8     | 2.40                     | 0.56              |
| 9:XI:15:ALA:HB2    | 9:XI:65:VAL:HG23   | 1.86                     | 0.56              |
| 26:YB:12:C:H2'     | 46:Y0:73:GLY:HA3   | 1.87                     | 0.56              |
| 25:YA:2632:A:HO2'  | 25:YA:2811:G:HO2'  | 1.51                     | 0.56              |
| 29:YF:107:LYS:HD2  | 29:YF:206:ILE:HA   | 1.86                     | 0.56              |
| 32:YI:33:ARG:HB3   | 32:YI:35:LEU:HG    | 1.86                     | 0.56              |
| 36:YQ:85:LYS:O     | 36:YQ:87:LYS:N     | 2.38                     | 0.56              |
| 45:YZ:77:ASP:OD2   | 45:YZ:80:ARG:HD3   | 2.05                     | 0.56              |
| 25:RA:1454:U:OP1   | 37:RR:77:ARG:NH1   | 2.34                     | 0.56              |
| 27:RD:108:PRO:HB3  | 27:RD:143:HIS:CE1  | 2.40                     | 0.56              |
| 27:RD:148:GLU:HB2  | 27:RD:151:LYS:HD2  | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:RY:81:LYS:HZ3   | 44:RY:98:VAL:HG11  | 1.69                     | 0.56              |
| 1:XA:1342:C:H4'    | 9:XI:125:TYR:HB3   | 1.87                     | 0.56              |
| 10:XJ:50:ILE:HD11  | 10:XJ:57:LYS:HD3   | 1.85                     | 0.56              |
| 50:Y4:71:ARG:HH11  | 50:Y4:71:ARG:HB2   | 1.68                     | 0.56              |
| 25:YA:1664:A:N6    | 25:YA:1996:C:H42   | 2.00                     | 0.56              |
| 3:QC:73:PRO:HG3    | 3:QC:105:GLU:HG3   | 1.88                     | 0.56              |
| 19:QS:64:GLU:HG3   | 50:R4:55:ARG:HH12  | 1.70                     | 0.56              |
| 25:RA:1316:U:H2'   | 25:RA:1317:A:C8    | 2.41                     | 0.56              |
| 28:RE:13:ARG:CB    | 28:RE:21:VAL:CG1   | 2.83                     | 0.56              |
| 29:RF:11:VAL:HG12  | 29:RF:12:LEU:H     | 1.69                     | 0.56              |
| 32:RI:116:LEU:O    | 32:RI:118:LYS:N    | 2.38                     | 0.56              |
| 1:XA:953:G:N7      | 13:XM:104:ARG:NH2  | 2.52                     | 0.56              |
| 25:YA:1798:U:H5''  | 27:YD:259:THR:HG22 | 1.87                     | 0.56              |
| 30:YG:81:LYS:O     | 30:YG:82:LEU:HB2   | 2.04                     | 0.56              |
| 45:YZ:19:ARG:NH1   | 45:YZ:84:GLU:O     | 2.35                     | 0.56              |
| 1:QA:501:C:H2'     | 1:QA:502:G:H8      | 1.69                     | 0.56              |
| 12:QL:117:ARG:HB3  | 12:QL:122:THR:HB   | 1.86                     | 0.56              |
| 35:RP:106:LEU:O    | 35:RP:107:LYS:HB2  | 2.05                     | 0.56              |
| 36:RQ:32:TYR:HE1   | 36:RQ:133:ARG:HG3  | 1.69                     | 0.56              |
| 36:RQ:24:GLY:O     | 36:RQ:26:TYR:N     | 2.36                     | 0.56              |
| 19:XS:5:LEU:HD11   | 50:Y4:67:TYR:H     | 1.69                     | 0.56              |
| 25:YA:1204:A:H1'   | 25:YA:1206:G:C8    | 2.40                     | 0.56              |
| 25:YA:1464:C:HO2'  | 25:YA:1528:A:H8    | 1.51                     | 0.56              |
| 25:YA:1991:U:H2'   | 25:YA:1992:G:H5''  | 1.87                     | 0.56              |
| 35:YP:101:VAL:HG23 | 35:YP:106:LEU:HB3  | 1.88                     | 0.56              |
| 26:YB:50:G:OP1     | 38:YS:61:ASN:ND2   | 2.38                     | 0.56              |
| 39:YT:60:THR:HG22  | 39:YT:77:PRO:HA    | 1.86                     | 0.56              |
| 41:YV:59:ALA:HB2   | 41:YV:96:ILE:HD13  | 1.88                     | 0.56              |
| 42:YW:71:VAL:HA    | 42:YW:107:LEU:HD12 | 1.87                     | 0.56              |
| 4:QD:195:ALA:CB    | 6:XF:16:GLN:O      | 2.51                     | 0.56              |
| 19:QS:41:VAL:HB    | 19:QS:42:PRO:CA    | 2.35                     | 0.56              |
| 25:RA:1337:G:OP2   | 43:RX:73:ARG:NH2   | 2.38                     | 0.56              |
| 25:RA:443:A:N7     | 29:RF:45:ARG:HD2   | 2.20                     | 0.56              |
| 28:RE:15:PHE:CD1   | 28:RE:20:ALA:CB    | 2.87                     | 0.56              |
| 25:RA:443:A:C5     | 29:RF:45:ARG:HD2   | 2.41                     | 0.56              |
| 32:RI:52:ARG:C     | 32:RI:56:LYS:H     | 2.03                     | 0.56              |
| 36:RQ:43:THR:HA    | 36:RQ:94:VAL:HG12  | 1.88                     | 0.56              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:HD11 | 1.87                     | 0.56              |
| 1:XA:403:C:OP1     | 4:XD:137:SER:OG    | 2.24                     | 0.56              |
| 1:XA:627:G:H2'     | 1:XA:628:G:H8      | 1.70                     | 0.56              |
| 27:YD:121:PRO:HA   | 27:YD:135:PHE:HD2  | 1.62                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:YI:79:ILE:HB    | 32:YI:142:VAL:HA  | 1.88                     | 0.56              |
| 45:YZ:152:ALA:HB2  | 45:YZ:168:GLU:HA  | 1.87                     | 0.56              |
| 1:QA:1004:A:O5'    | 1:QA:1025:U:N3    | 2.38                     | 0.56              |
| 1:QA:613:C:H42     | 1:QA:627:G:H1     | 1.53                     | 0.56              |
| 17:QQ:90:ILE:O     | 17:QQ:94:ASN:ND2  | 2.38                     | 0.56              |
| 25:RA:2212:A:H1'   | 25:RA:2215:G:C5   | 2.40                     | 0.56              |
| 28:RE:10:GLY:HA3   | 39:RT:8:LYS:HD2   | 1.85                     | 0.56              |
| 36:RQ:66:ILE:HA    | 36:RQ:104:PHE:HA  | 1.87                     | 0.56              |
| 37:RR:67:LEU:HD13  | 37:RR:76:VAL:HG21 | 1.86                     | 0.56              |
| 41:RV:44:LYS:HE2   | 41:RV:45:THR:H    | 1.70                     | 0.56              |
| 1:XA:235:C:H2'     | 1:XA:236:G:H8     | 1.70                     | 0.56              |
| 1:XA:720:C:H5''    | 18:XR:52:PRO:HA   | 1.88                     | 0.56              |
| 4:QD:195:ALA:HB2   | 6:XF:20:ALA:CB    | 2.35                     | 0.56              |
| 30:YG:67:LYS:HZ1   | 50:Y4:6:HIS:CD2   | 2.23                     | 0.56              |
| 36:YQ:20:ALA:HB3   | 45:YZ:79:ARG:CZ   | 2.35                     | 0.56              |
| 1:QA:6:G:H4'       | 1:QA:298:A:H4'    | 1.87                     | 0.56              |
| 1:QA:376:G:H5''    | 16:QP:5:ARG:HD2   | 1.87                     | 0.56              |
| 1:QA:942:G:N2      | 9:QI:124:GLN:OE1  | 2.31                     | 0.56              |
| 35:RP:68:GLN:HG2   | 54:R8:12:LYS:HD3  | 1.88                     | 0.56              |
| 25:RA:1012:U:O2'   | 25:RA:1013:C:OP2  | 2.19                     | 0.56              |
| 25:RA:2019:A:OP2   | 51:R5:9:LYS:NZ    | 2.39                     | 0.56              |
| 28:RE:4:ILE:HD12   | 28:RE:28:ALA:HB1  | 1.88                     | 0.56              |
| 45:RZ:111:VAL:HG13 | 45:RZ:112:ARG:N   | 2.19                     | 0.56              |
| 1:XA:971:G:H5''    | 1:XA:972:C:H5''   | 1.88                     | 0.56              |
| 51:Y5:33:CYS:SG    | 51:Y5:34:PRO:HD2  | 2.45                     | 0.56              |
| 25:YA:2689:U:OP2   | 25:YA:2719:G:N2   | 2.33                     | 0.56              |
| 26:YB:24:G:H1'     | 26:YB:26:A:H62    | 1.70                     | 0.56              |
| 31:YH:153:LYS:HA   | 31:YH:153:LYS:NZ  | 2.21                     | 0.56              |
| 41:YV:66:ARG:HH11  | 41:YV:88:ARG:HD3  | 1.71                     | 0.56              |
| 23:QW:18:G:H22     | 23:QW:55:U:H1'    | 1.71                     | 0.56              |
| 51:R5:50:GLY:HA3   | 51:R5:56:LYS:CG   | 2.35                     | 0.56              |
| 32:RI:8:PRO:HD3    | 32:RI:15:VAL:HG13 | 1.87                     | 0.56              |
| 52:Y6:25:LYS:HE2   | 52:Y6:27:LYS:HE3  | 1.87                     | 0.56              |
| 25:YA:1266:G:O5'   | 42:YW:15:ARG:NH2  | 2.38                     | 0.56              |
| 25:YA:2820:A:C8    | 28:YE:109:LYS:HE2 | 2.40                     | 0.56              |
| 31:YH:92:ILE:HD12  | 31:YH:92:ILE:H    | 1.71                     | 0.56              |
| 2:QB:82:ARG:HA     | 2:QB:92:TYR:HE2   | 1.71                     | 0.56              |
| 8:QH:106:GLY:O     | 8:QH:122:ARG:NH2  | 2.36                     | 0.56              |
| 10:QJ:5:ARG:HG3    | 10:QJ:71:LEU:HD11 | 1.87                     | 0.56              |
| 12:QL:45:PRO:HB3   | 12:QL:92:ASP:HB3  | 1.87                     | 0.56              |
| 25:RA:27:G:O2'     | 25:RA:28:A:O5'    | 2.23                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:RI:29:TYR:HD2  | 32:RI:30:LEU:HD23  | 1.71                     | 0.56              |
| 1:XA:1356:G:H2'   | 1:XA:1357:A:C8     | 2.40                     | 0.56              |
| 1:XA:1347:G:N2    | 1:XA:1374:A:OP2    | 2.34                     | 0.56              |
| 2:XB:84:GLU:HB3   | 2:XB:219:VAL:HG21  | 1.86                     | 0.56              |
| 3:XC:174:PRO:HD2  | 3:XC:182:ILE:HD11  | 1.88                     | 0.56              |
| 7:XG:54:THR:O     | 7:XG:56:GLN:N      | 2.39                     | 0.56              |
| 16:XP:20:VAL:HG21 | 16:XP:32:TYR:CD2   | 2.40                     | 0.56              |
| 25:YA:2109:U:H3   | 25:YA:2180:U:H3    | 1.54                     | 0.56              |
| 34:YO:97:ARG:HA   | 34:YO:117:LEU:HD22 | 1.88                     | 0.56              |
| 25:RA:242:G:C8    | 54:R8:5:LYS:HG2    | 2.40                     | 0.56              |
| 25:RA:2690:C:OP2  | 37:RR:14:SER:HB3   | 2.06                     | 0.56              |
| 1:XA:1128:C:N4    | 1:XA:1144:G:N1     | 2.54                     | 0.56              |
| 1:XA:911:U:OP2    | 12:XL:97:ARG:NH2   | 2.27                     | 0.56              |
| 2:XB:21:ARG:O     | 2:XB:23:ARG:HD3    | 2.05                     | 0.56              |
| 4:XD:122:ARG:NH1  | 4:XD:134:ASP:O     | 2.39                     | 0.56              |
| 25:YA:2849:U:OP2  | 39:YT:95:ARG:NH1   | 2.39                     | 0.56              |
| 27:YD:43:ARG:NH1  | 27:YD:44:ASN:OD1   | 2.39                     | 0.56              |
| 31:YH:10:PRO:HD2  | 31:YH:50:VAL:CG1   | 2.35                     | 0.56              |
| 33:YN:56:ASN:N    | 33:YN:125:GLY:O    | 2.22                     | 0.56              |
| 44:YY:95:LYS:HB3  | 44:YY:100:ALA:HA   | 1.87                     | 0.56              |
| 1:QA:620:C:C2     | 4:QD:135:LEU:HG    | 2.40                     | 0.56              |
| 4:QD:165:MET:SD   | 4:QD:168:ARG:HD2   | 2.46                     | 0.56              |
| 1:QA:974:A:H1'    | 14:QN:31:ARG:HE    | 1.70                     | 0.56              |
| 51:R5:55:ARG:HH12 | 51:R5:57:VAL:HA    | 1.69                     | 0.56              |
| 25:RA:1509:C:H3'  | 25:RA:1510:A:H5''  | 1.88                     | 0.56              |
| 25:RA:1754:C:OP1  | 39:RT:96:ARG:NH1   | 2.34                     | 0.56              |
| 25:RA:793:A:OP2   | 25:RA:2071:A:O2'   | 2.22                     | 0.56              |
| 32:RI:41:GLU:HA   | 32:RI:44:LEU:HB2   | 1.87                     | 0.56              |
| 43:RX:31:HIS:CD2  | 43:RX:32:PRO:HD2   | 2.41                     | 0.56              |
| 45:RZ:182:LYS:H   | 45:RZ:182:LYS:HD3  | 1.70                     | 0.56              |
| 1:XA:250:A:H4'    | 1:XA:251:G:O5'     | 2.04                     | 0.56              |
| 3:XC:130:VAL:O    | 3:XC:134:ILE:HG12  | 2.06                     | 0.56              |
| 4:XD:11:LEU:HD13  | 4:XD:66:ARG:HG2    | 1.87                     | 0.56              |
| 25:YA:2335:A:O2'  | 25:YA:2336:A:H2'   | 2.05                     | 0.56              |
| 25:YA:2340:G:H2'  | 25:YA:2341:G:H8    | 1.70                     | 0.56              |
| 12:QL:89:ARG:HB3  | 12:QL:97:ARG:HA    | 1.88                     | 0.55              |
| 51:R5:52:TYR:O    | 51:R5:53:ALA:HB2   | 2.06                     | 0.55              |
| 52:R6:36:LEU:HB2  | 52:R6:50:ARG:HA    | 1.89                     | 0.55              |
| 29:RF:24:LEU:CD2  | 29:RF:115:ALA:HA   | 2.36                     | 0.55              |
| 35:RP:121:LYS:HD3 | 35:RP:122:PRO:HD2  | 1.88                     | 0.55              |
| 39:RT:26:ASP:O    | 39:RT:49:VAL:HG12  | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1175:G:H2'    | 1:XA:1176:A:C8     | 2.41                     | 0.55              |
| 3:XC:9:GLY:HA2     | 3:XC:12:LEU:HD23   | 1.88                     | 0.55              |
| 25:YA:1266:G:O2'   | 25:YA:2012:G:O6    | 2.16                     | 0.55              |
| 38:YS:58:LEU:HD23  | 38:YS:58:LEU:H     | 1.70                     | 0.55              |
| 33:YN:40:PRO:O     | 40:YU:64:ARG:HD2   | 2.06                     | 0.55              |
| 4:QD:187:ARG:NH2   | 4:QD:193:ASP:OD2   | 2.38                     | 0.55              |
| 23:QW:12:U:H3      | 23:QW:23:A:N6      | 2.02                     | 0.55              |
| 50:R4:24:THR:OG1   | 50:R4:25:TYR:N     | 2.38                     | 0.55              |
| 29:RF:110:LEU:HD11 | 29:RF:181:LEU:HD12 | 1.88                     | 0.55              |
| 32:RI:92:VAL:HG13  | 32:RI:120:ILE:HG23 | 1.88                     | 0.55              |
| 25:RA:2404:C:H1'   | 35:RP:67:MET:HE1   | 1.88                     | 0.55              |
| 1:XA:486:U:H2'     | 1:XA:487:A:H8      | 1.70                     | 0.55              |
| 2:XB:158:LEU:HD13  | 2:XB:182:ILE:HD11  | 1.89                     | 0.55              |
| 39:YT:29:ARG:HB2   | 39:YT:46:GLU:HG3   | 1.88                     | 0.55              |
| 1:QA:411:A:H62     | 1:QA:413:G:H21     | 1.53                     | 0.55              |
| 2:QB:5:ILE:HD12    | 2:QB:224:GLN:HG2   | 1.88                     | 0.55              |
| 2:QB:71:VAL:HG12   | 2:QB:93:VAL:HB     | 1.88                     | 0.55              |
| 10:QJ:16:LEU:HD23  | 10:QJ:94:VAL:HG13  | 1.89                     | 0.55              |
| 47:R1:53:VAL:HG11  | 47:R1:90:ILE:HD11  | 1.88                     | 0.55              |
| 19:QS:64:GLU:HG3   | 50:R4:55:ARG:NH1   | 2.21                     | 0.55              |
| 25:RA:1417:C:H2'   | 25:RA:1418:G:O4'   | 2.05                     | 0.55              |
| 28:RE:63:LEU:CD1   | 28:RE:65:GLY:H     | 2.20                     | 0.55              |
| 1:XA:664:G:N2      | 1:XA:741:G:H1      | 2.03                     | 0.55              |
| 10:XJ:34:VAL:HG22  | 10:XJ:74:ILE:HG22  | 1.89                     | 0.55              |
| 15:XO:18:PHE:CE1   | 15:XO:21:ASP:HB2   | 2.41                     | 0.55              |
| 27:YD:232:PRO:HB3  | 27:YD:244:ARG:NH1  | 2.21                     | 0.55              |
| 35:YP:52:GLU:HG3   | 35:YP:57:THR:HG22  | 1.88                     | 0.55              |
| 36:YQ:20:ALA:HB3   | 45:YZ:79:ARG:NH2   | 2.21                     | 0.55              |
| 39:YT:39:ARG:HG2   | 39:YT:40:THR:H     | 1.72                     | 0.55              |
| 41:YV:38:LEU:H     | 41:YV:51:VAL:HG13  | 1.70                     | 0.55              |
| 1:QA:1118:C:H1'    | 1:QA:1179:A:C4     | 2.41                     | 0.55              |
| 10:QJ:78:ASN:O     | 10:QJ:81:THR:OG1   | 2.24                     | 0.55              |
| 13:QM:80:ARG:CD    | 50:R4:71:ARG:NH2   | 2.48                     | 0.55              |
| 32:RI:21:VAL:HG21  | 32:RI:25:TYR:HD2   | 1.71                     | 0.55              |
| 32:RI:52:ARG:O     | 32:RI:56:LYS:CA    | 2.55                     | 0.55              |
| 34:RO:78:ARG:HH21  | 39:RT:103:ARG:NH2  | 2.03                     | 0.55              |
| 41:RV:7:THR:HG23   | 41:RV:22:VAL:HG11  | 1.88                     | 0.55              |
| 42:RW:86:LEU:HD22  | 42:RW:96:ILE:HD11  | 1.88                     | 0.55              |
| 54:Y8:50:LEU:HD12  | 54:Y8:51:ALA:N     | 2.21                     | 0.55              |
| 25:YA:922:U:H2'    | 25:YA:923:C:C6     | 2.42                     | 0.55              |
| 29:YF:101:LEU:O    | 29:YF:106:ARG:NH1  | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:121:ILE:HG12 | 31:YH:140:LYS:HD2  | 1.89                     | 0.55              |
| 1:QA:437:U:H2'     | 1:QA:438:G:O4'     | 2.06                     | 0.55              |
| 4:QD:195:ALA:HB3   | 6:XF:20:ALA:HB2    | 1.87                     | 0.55              |
| 8:QH:86:ILE:HG13   | 8:QH:133:LEU:HD22  | 1.89                     | 0.55              |
| 51:R5:4:HIS:HB3    | 51:R5:5:PRO:CD     | 2.32                     | 0.55              |
| 25:RA:2015:A:H1'   | 51:R5:2:ALA:HA     | 1.87                     | 0.55              |
| 25:RA:181:A:H1'    | 25:RA:435:C:H5'    | 1.88                     | 0.55              |
| 29:RF:101:LEU:O    | 29:RF:106:ARG:NH1  | 2.40                     | 0.55              |
| 32:RI:94:ALA:H     | 32:RI:116:LEU:HD13 | 1.71                     | 0.55              |
| 44:RY:95:LYS:CB    | 44:RY:100:ALA:HA   | 2.36                     | 0.55              |
| 44:RY:81:LYS:HB2   | 44:RY:96:ILE:HG22  | 1.89                     | 0.55              |
| 4:XD:31:CYS:SG     | 4:XD:31:CYS:O      | 2.65                     | 0.55              |
| 5:XE:37:ARG:HA     | 5:XE:114:GLY:N     | 2.21                     | 0.55              |
| 1:XA:1226:C:O2'    | 13:XM:103:THR:O    | 2.23                     | 0.55              |
| 20:XT:49:ALA:HB1   | 20:XT:99:LEU:HB2   | 1.89                     | 0.55              |
| 25:YA:1416:G:H2'   | 25:YA:1417:C:C6    | 2.42                     | 0.55              |
| 25:YA:2096:U:H3    | 25:YA:2193:G:H1    | 1.54                     | 0.55              |
| 25:YA:2688:U:H5    | 25:YA:2720:U:OP2   | 1.89                     | 0.55              |
| 4:QD:30:LYS:O      | 4:QD:30:LYS:HG2    | 2.07                     | 0.55              |
| 9:QI:77:ILE:O      | 9:QI:81:ILE:HG12   | 2.06                     | 0.55              |
| 50:R4:16:CYS:SG    | 50:R4:36:CYS:N     | 2.79                     | 0.55              |
| 25:RA:1045:A:N9    | 25:RA:1111:A:N6    | 2.55                     | 0.55              |
| 25:RA:1141:U:H1'   | 25:RA:1142(A):A:C6 | 2.42                     | 0.55              |
| 27:RD:35:LYS:NZ    | 27:RD:104:TYR:HB2  | 2.21                     | 0.55              |
| 25:RA:535:C:O3'    | 40:RU:53:ARG:NH1   | 2.39                     | 0.55              |
| 44:RY:96:ILE:HG12  | 44:RY:101:LYS:HB2  | 1.88                     | 0.55              |
| 2:XB:82:ARG:NH1    | 2:XB:86:GLU:OE2    | 2.40                     | 0.55              |
| 25:YA:273(C):C:H42 | 25:YA:363(C):G:H1  | 1.52                     | 0.55              |
| 26:YB:13:A:N1      | 26:YB:69:G:O2'     | 2.28                     | 0.55              |
| 25:YA:1826:G:OP1   | 27:YD:224:ALA:N    | 2.39                     | 0.55              |
| 28:YE:14:ILE:CG2   | 28:YE:21:VAL:HG21  | 2.34                     | 0.55              |
| 28:YE:63:LEU:HD12  | 28:YE:64:LYS:N     | 2.22                     | 0.55              |
| 32:YI:129:THR:HA   | 32:YI:137:PRO:HA   | 1.88                     | 0.55              |
| 39:YT:3:ARG:HG3    | 39:YT:7:ILE:HG12   | 1.88                     | 0.55              |
| 1:QA:1047:G:H1     | 1:QA:1210:C:H42    | 1.55                     | 0.55              |
| 25:RA:1316:U:H2'   | 25:RA:1317:A:H8    | 1.71                     | 0.55              |
| 25:RA:2805:G:H2'   | 25:RA:2807:G:C8    | 2.41                     | 0.55              |
| 40:RU:52:ARG:HA    | 40:RU:55:ARG:HG3   | 1.87                     | 0.55              |
| 44:RY:37:VAL:HG21  | 44:RY:72:VAL:HG21  | 1.88                     | 0.55              |
| 1:XA:1128:C:C2     | 1:XA:1144:G:N2     | 2.74                     | 0.55              |
| 1:XA:1414:U:H2'    | 1:XA:1415:G:C8     | 2.42                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:362:G:N2     | 1:XA:365:U:OP2     | 2.39                     | 0.55              |
| 3:QC:79:ARG:HD2   | 11:XK:99:GLN:CD    | 2.27                     | 0.55              |
| 52:Y6:28:ARG:HB3  | 52:Y6:30:THR:H     | 1.71                     | 0.55              |
| 25:YA:2438:U:O3'  | 25:YA:2439:A:H3'   | 2.07                     | 0.55              |
| 25:YA:2757:A:OP1  | 55:Y9:19:ARG:HA    | 2.06                     | 0.55              |
| 25:YA:458:G:O2'   | 25:YA:469:G:O6     | 2.19                     | 0.55              |
| 25:YA:574:C:N3    | 28:YE:145:LYS:NZ   | 2.50                     | 0.55              |
| 29:YF:68:LYS:O    | 29:YF:69:HIS:HB2   | 2.07                     | 0.55              |
| 31:YH:157:TYR:HA  | 31:YH:171:LEU:O    | 2.06                     | 0.55              |
| 31:YH:41:MET:HE1  | 31:YH:64:LEU:HB3   | 1.87                     | 0.55              |
| 1:QA:1159:U:O2'   | 1:QA:1160:G:N7     | 2.39                     | 0.55              |
| 19:QS:42:PRO:CD   | 50:R4:63:TYR:CE1   | 2.89                     | 0.55              |
| 25:RA:807:U:H2'   | 25:RA:808:G:C8     | 2.41                     | 0.55              |
| 13:QM:7:VAL:HB    | 30:RG:115:ARG:HH12 | 1.71                     | 0.55              |
| 36:RQ:30:GLY:CA   | 36:RQ:107:ALA:HB2  | 2.37                     | 0.55              |
| 1:XA:410:G:H4'    | 1:XA:411:A:OP1     | 2.07                     | 0.55              |
| 5:XE:50:GLU:HB3   | 5:XE:53:LEU:HD13   | 1.88                     | 0.55              |
| 8:XH:86:ILE:HG22  | 8:XH:93:VAL:HG21   | 1.89                     | 0.55              |
| 9:XI:16:ARG:HB2   | 9:XI:64:THR:HB     | 1.89                     | 0.55              |
| 1:XA:1226:C:O2'   | 13:XM:111:LYS:NZ   | 2.40                     | 0.55              |
| 46:Y0:27:GLU:HB2  | 46:Y0:69:PHE:HD1   | 1.72                     | 0.55              |
| 25:YA:1062:G:H2'  | 25:YA:1063:G:C8    | 2.42                     | 0.55              |
| 41:YV:61:VAL:HG23 | 41:YV:63:GLY:H     | 1.71                     | 0.55              |
| 1:QA:115:G:H4'    | 1:QA:116:A:O5'     | 2.07                     | 0.55              |
| 1:QA:1162:C:H2'   | 1:QA:1163:C:O4'    | 2.07                     | 0.55              |
| 1:QA:1405:G:OP2   | 58:QA:1667:PAR:O34 | 2.25                     | 0.55              |
| 31:RH:109:PHE:HZ  | 31:RH:152:ARG:HG2  | 1.72                     | 0.55              |
| 11:XK:34:ASP:OD1  | 11:XK:38:ASN:N     | 2.39                     | 0.55              |
| 23:XW:20:U:H2'    | 23:XW:21:A:H4'     | 1.88                     | 0.55              |
| 25:YA:1178:C:H2'  | 25:YA:1179:C:C6    | 2.41                     | 0.55              |
| 25:YA:1359:A:H61  | 25:YA:1372:U:H3    | 1.39                     | 0.55              |
| 32:YI:3:VAL:HG12  | 32:YI:38:LEU:HA    | 1.87                     | 0.55              |
| 35:YP:71:VAL:HG13 | 35:YP:72:PRO:HD3   | 1.88                     | 0.55              |
| 39:YT:26:ASP:O    | 39:YT:49:VAL:HG12  | 2.07                     | 0.55              |
| 41:YV:34:GLU:O    | 41:YV:36:PRO:HD3   | 2.06                     | 0.55              |
| 42:YW:14:PRO:O    | 42:YW:17:VAL:N     | 2.40                     | 0.55              |
| 1:QA:976:G:OP2    | 1:QA:1358:U:O2'    | 2.25                     | 0.55              |
| 10:QJ:8:LEU:HB3   | 10:QJ:16:LEU:HD21  | 1.87                     | 0.55              |
| 14:QN:48:ALA:HB2  | 14:QN:53:LEU:HD12  | 1.89                     | 0.55              |
| 25:RA:1689:A:H2'  | 25:RA:1690:A:H8    | 1.72                     | 0.55              |
| 29:RF:24:LEU:HG   | 29:RF:115:ALA:CB   | 2.37                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:RH:124:GLU:HB3  | 31:RH:132:ARG:HG3   | 1.89                     | 0.55              |
| 39:RT:1:MET:O      | 39:RT:3:ARG:N       | 2.40                     | 0.55              |
| 8:XH:54:ASP:OD1    | 8:XH:54:ASP:N       | 2.39                     | 0.55              |
| 12:XL:70:ILE:HG12  | 12:XL:100:ILE:HD12  | 1.88                     | 0.55              |
| 54:Y8:60:LEU:HB3   | 54:Y8:63:PRO:HG2    | 1.89                     | 0.55              |
| 29:YF:116:ASP:OD2  | 35:YP:1:MET:N       | 2.26                     | 0.55              |
| 39:YT:62:THR:HG22  | 39:YT:75:ILE:HG12   | 1.89                     | 0.55              |
| 5:QE:78:HIS:CE1    | 5:QE:142:LEU:HD23   | 2.42                     | 0.54              |
| 10:QJ:13:HIS:CE1   | 10:QJ:14:LYS:HE3    | 2.42                     | 0.54              |
| 14:QN:24:CYS:HB3   | 14:QN:28:GLY:H      | 1.71                     | 0.54              |
| 48:R2:42:GLY:O     | 48:R2:44:LEU:N      | 2.35                     | 0.54              |
| 25:RA:1021:A:N6    | 25:RA:1142(A):A:H61 | 2.02                     | 0.54              |
| 25:RA:1359:A:N6    | 25:RA:1372:U:C4     | 2.75                     | 0.54              |
| 25:RA:2335:A:O2'   | 25:RA:2336:A:H2'    | 2.07                     | 0.54              |
| 29:RF:184:TYR:CE2  | 29:RF:188:ARG:HD2   | 2.42                     | 0.54              |
| 36:RQ:31:ASP:O     | 36:RQ:134:ARG:HB2   | 2.07                     | 0.54              |
| 4:XD:92:VAL:O      | 4:XD:96:LEU:HD22    | 2.07                     | 0.54              |
| 5:XE:100:VAL:HG22  | 5:XE:118:ILE:HG22   | 1.89                     | 0.54              |
| 10:XJ:33:GLN:HB2   | 10:XJ:75:ILE:HD11   | 1.88                     | 0.54              |
| 23:XW:16:U:H3'     | 23:XW:17:C:H5'      | 1.89                     | 0.54              |
| 45:YZ:48:PHE:CE1   | 45:YZ:52:SER:HA     | 2.42                     | 0.54              |
| 1:QA:1321:C:H3'    | 1:QA:1322:C:H5''    | 1.88                     | 0.54              |
| 5:QE:7:GLU:N       | 5:QE:35:GLY:O       | 2.36                     | 0.54              |
| 54:R8:29:LYS:HD3   | 54:R8:44:LYS:HB2    | 1.88                     | 0.54              |
| 25:RA:1085:A:O2'   | 25:RA:1086:A:OP1    | 2.24                     | 0.54              |
| 25:RA:622:G:OP2    | 35:RP:108:LYS:NZ    | 2.29                     | 0.54              |
| 26:RB:38:C:N3      | 26:RB:44:G:N2       | 2.42                     | 0.54              |
| 33:RN:30:ILE:HG22  | 33:RN:34:LEU:HD22   | 1.88                     | 0.54              |
| 43:RX:25:LYS:HD3   | 43:RX:80:ILE:HD11   | 1.89                     | 0.54              |
| 1:XA:963:G:N2      | 1:XA:972:C:C2       | 2.70                     | 0.54              |
| 25:YA:2346:A:H8    | 54:Y8:35:GLN:NE2    | 2.05                     | 0.54              |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:H8   | 1.73                     | 0.54              |
| 25:YA:34:C:H41     | 25:YA:447:A:H61     | 1.55                     | 0.54              |
| 25:YA:898:C:H2'    | 25:YA:899:A:H5'     | 1.88                     | 0.54              |
| 27:YD:12:SER:O     | 27:YD:16:MET:HB2    | 2.08                     | 0.54              |
| 25:YA:764:A:N3     | 27:YD:213:ARG:NH1   | 2.55                     | 0.54              |
| 33:YN:42:TRP:O     | 40:YU:64:ARG:NH2    | 2.41                     | 0.54              |
| 25:YA:1187:G:H5''  | 41:YV:81:TYR:CE1    | 2.43                     | 0.54              |
| 45:YZ:5:LEU:HD21   | 45:YZ:44:PHE:HA     | 1.89                     | 0.54              |
| 9:QI:26:VAL:HG22   | 9:QI:61:ALA:HB3     | 1.89                     | 0.54              |
| 22:QV:21:A:H61     | 22:QV:46:G:H2'      | 1.73                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:R5:55:ARG:HH11  | 51:R5:57:VAL:CA    | 2.20                     | 0.54              |
| 25:RA:686:G:H21    | 25:RA:788:A:H61    | 1.54                     | 0.54              |
| 36:RQ:54:MET:HG3   | 36:RQ:117:ALA:HB1  | 1.89                     | 0.54              |
| 33:RN:40:PRO:HB3   | 40:RU:68:ALA:HB2   | 1.89                     | 0.54              |
| 1:XA:1151:A:H2'    | 1:XA:1152:A:C8     | 2.43                     | 0.54              |
| 3:XC:150:LYS:HE2   | 3:XC:152:ILE:HD11  | 1.88                     | 0.54              |
| 12:XL:115:LYS:O    | 12:XL:117:ARG:N    | 2.35                     | 0.54              |
| 13:XM:22:ILE:HD12  | 13:XM:25:ILE:HD12  | 1.89                     | 0.54              |
| 25:YA:587:C:H4'    | 25:YA:588:U:O5'    | 2.07                     | 0.54              |
| 37:YR:56:LYS:NZ    | 37:YR:87:TYR:O     | 2.40                     | 0.54              |
| 37:YR:55:ALA:HB2   | 37:YR:79:LEU:HD13  | 1.89                     | 0.54              |
| 4:QD:149:ALA:HB3   | 4:QD:152:SER:HB2   | 1.89                     | 0.54              |
| 25:RA:307:G:H21    | 25:RA:330:A:H62    | 1.55                     | 0.54              |
| 25:RA:442:G:H1'    | 29:RF:48:THR:HG21  | 1.89                     | 0.54              |
| 27:RD:35:LYS:HZ1   | 27:RD:104:TYR:HB2  | 1.71                     | 0.54              |
| 28:RE:35:GLN:HE21  | 28:RE:37:ARG:CZ    | 2.21                     | 0.54              |
| 32:RI:113:ARG:HG3  | 32:RI:131:LYS:NZ   | 2.23                     | 0.54              |
| 45:RZ:146:ILE:HA   | 45:RZ:174:VAL:HB   | 1.90                     | 0.54              |
| 1:XA:910:C:P       | 12:XL:97:ARG:HH22  | 2.31                     | 0.54              |
| 1:XA:973:G:H3'     | 1:XA:974:A:H5''    | 1.88                     | 0.54              |
| 18:XR:31:LEU:H     | 18:XR:31:LEU:HD23  | 1.73                     | 0.54              |
| 51:Y5:55:ARG:HG3   | 51:Y5:57:VAL:H     | 1.73                     | 0.54              |
| 25:YA:2349:G:OP2   | 54:Y8:42:ARG:HD3   | 2.08                     | 0.54              |
| 25:YA:27:G:N2      | 25:YA:513:A:OP2    | 2.40                     | 0.54              |
| 25:YA:900:A:H3'    | 25:YA:901:A:H8     | 1.73                     | 0.54              |
| 35:YP:64:LYS:O     | 35:YP:66:GLY:N     | 2.41                     | 0.54              |
| 36:YQ:109:VAL:HG13 | 36:YQ:113:GLN:HB3  | 1.89                     | 0.54              |
| 1:QA:1126:U:H1'    | 1:QA:1280:A:N7     | 2.23                     | 0.54              |
| 30:RG:16:ARG:NH2   | 30:RG:28:VAL:O     | 2.41                     | 0.54              |
| 32:RI:93:THR:O     | 32:RI:97:ILE:HG12  | 2.06                     | 0.54              |
| 1:XA:1095:U:P      | 1:XA:1108:G:H1     | 2.30                     | 0.54              |
| 5:XE:12:LEU:HD21   | 5:XE:14:ARG:HD3    | 1.89                     | 0.54              |
| 10:XJ:9:ARG:HB2    | 10:XJ:95:GLU:HB3   | 1.88                     | 0.54              |
| 48:Y2:35:LEU:HD12  | 48:Y2:53:LEU:HD12  | 1.89                     | 0.54              |
| 25:YA:1798:U:H5'   | 27:YD:259:THR:HG22 | 1.90                     | 0.54              |
| 1:QA:983:A:N1      | 1:QA:1222:G:N2     | 2.56                     | 0.54              |
| 9:QI:121:ARG:NH1   | 9:QI:122:ALA:O     | 2.40                     | 0.54              |
| 47:R1:58:ILE:HD11  | 47:R1:86:SER:HB2   | 1.88                     | 0.54              |
| 48:R2:50:ILE:HD12  | 48:R2:51:ARG:H     | 1.73                     | 0.54              |
| 25:RA:642:G:H21    | 25:RA:646:A:H2     | 1.55                     | 0.54              |
| 37:RR:103:ARG:NH1  | 37:RR:108:GLY:O    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2292:C:OP1  | 38:RS:17:ARG:NH2   | 2.40                     | 0.54              |
| 40:RU:112:ARG:NH2 | 41:RV:47:VAL:HG13  | 2.23                     | 0.54              |
| 43:RX:83:VAL:CG1  | 43:RX:87:GLN:HB2   | 2.38                     | 0.54              |
| 45:RZ:53:ILE:H    | 45:RZ:71:VAL:HG13  | 1.72                     | 0.54              |
| 3:XC:150:LYS:HB3  | 3:XC:201:TYR:HB2   | 1.90                     | 0.54              |
| 7:XG:49:ILE:O     | 7:XG:53:LYS:HB3    | 2.07                     | 0.54              |
| 46:Y0:20:ARG:O    | 46:Y0:24:LYS:NZ    | 2.39                     | 0.54              |
| 26:YB:43:C:H5'    | 50:Y4:1:MET:HA     | 1.89                     | 0.54              |
| 25:YA:99:U:H4'    | 25:YA:101:G:H5''   | 1.89                     | 0.54              |
| 25:YA:2573:C:OP1  | 25:YA:2574:G:OP1   | 2.25                     | 0.54              |
| 33:YN:35:ARG:HB2  | 33:YN:42:TRP:CH2   | 2.42                     | 0.54              |
| 25:RA:1453:A:N6   | 25:RA:2702:U:H1'   | 2.23                     | 0.54              |
| 25:RA:2068:U:N3   | 25:RA:2430:A:H2    | 2.04                     | 0.54              |
| 25:RA:78:A:H2'    | 25:RA:79:G:H8      | 1.73                     | 0.54              |
| 26:RB:44:G:H1'    | 26:RB:47:C:H42     | 1.71                     | 0.54              |
| 35:RP:38:GLN:HG2  | 35:RP:45:LEU:CD1   | 2.36                     | 0.54              |
| 26:RB:52:A:N6     | 38:RS:33:LYS:HG3   | 2.23                     | 0.54              |
| 39:RT:111:ARG:O   | 39:RT:112:ARG:HG3  | 2.08                     | 0.54              |
| 1:XA:299:G:H2'    | 1:XA:300:A:C8      | 2.43                     | 0.54              |
| 7:XG:20:ASP:HB3   | 7:XG:23:VAL:HG23   | 1.89                     | 0.54              |
| 50:Y4:55:ARG:HG3  | 50:Y4:59:PHE:HD2   | 1.72                     | 0.54              |
| 25:YA:444:C:H4'   | 29:YF:49:ALA:HB2   | 1.89                     | 0.54              |
| 25:YA:2061:G:OP1  | 29:YF:68:LYS:NZ    | 2.41                     | 0.54              |
| 40:YU:76:TYR:CZ   | 40:YU:80:ILE:HG13  | 2.43                     | 0.54              |
| 1:QA:1453:G:H8    | 20:QT:39:LYS:HZ1   | 1.55                     | 0.54              |
| 1:QA:1499:A:OP1   | 1:QA:1505:G:OP2    | 2.26                     | 0.54              |
| 25:RA:1359:A:C6   | 25:RA:1372:U:C4    | 2.96                     | 0.54              |
| 35:RP:14:LYS:O    | 35:RP:16:ARG:HG2   | 2.08                     | 0.54              |
| 13:XM:3:ARG:HA    | 13:XM:9:ILE:CG2    | 2.37                     | 0.54              |
| 25:YA:1790:C:H2'  | 25:YA:1791:A:C5    | 2.42                     | 0.54              |
| 30:YG:15:VAL:HG21 | 30:YG:176:LEU:HD23 | 1.90                     | 0.54              |
| 1:QA:1305:G:N2    | 1:QA:1331:G:H2'    | 2.22                     | 0.54              |
| 1:QA:1436:U:H2'   | 1:QA:1437:C:O4'    | 2.07                     | 0.54              |
| 13:QM:22:ILE:HB   | 13:QM:25:ILE:HD12  | 1.89                     | 0.54              |
| 23:QW:68:C:H2'    | 23:QW:69:G:H8      | 1.71                     | 0.54              |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:C8    | 2.43                     | 0.54              |
| 25:RA:2543:G:H21  | 25:RA:2646:C:H5''  | 1.73                     | 0.54              |
| 45:RZ:82:ARG:HG3  | 45:RZ:83:PRO:HD2   | 1.90                     | 0.54              |
| 3:XC:15:THR:HG23  | 3:XC:181:ASN:HD22  | 1.73                     | 0.54              |
| 16:XP:43:LYS:HG2  | 16:XP:48:TRP:CE3   | 2.42                     | 0.54              |
| 23:XW:49:C:N3     | 23:XW:65:G:N2      | 2.55                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:YE:111:ARG:HD2 | 28:YE:160:TYR:CD2 | 2.42                     | 0.54              |
| 31:YH:12:PRO:CD   | 31:YH:48:GLY:O    | 2.55                     | 0.54              |
| 45:YZ:149:SER:HB2 | 45:YZ:172:ALA:O   | 2.07                     | 0.54              |
| 1:QA:412:A:H4'    | 1:QA:413:G:O5'    | 2.08                     | 0.54              |
| 2:QB:204:ASN:HD22 | 2:QB:206:ASP:H    | 1.56                     | 0.54              |
| 2:QB:235:SER:O    | 2:QB:237:ALA:N    | 2.41                     | 0.54              |
| 19:QS:10:PHE:HE1  | 19:QS:16:LEU:HD22 | 1.73                     | 0.54              |
| 13:QM:80:ARG:HB2  | 50:R4:71:ARG:HH22 | 1.72                     | 0.54              |
| 25:RA:1268:A:H2'  | 25:RA:1269:A:O4'  | 2.07                     | 0.54              |
| 25:RA:2441:C:OP2  | 25:RA:2586:C:O2'  | 2.25                     | 0.54              |
| 25:RA:2725:A:O2'  | 25:RA:2726:U:H5'' | 2.08                     | 0.54              |
| 25:RA:288:C:H2'   | 25:RA:289:A:C8    | 2.42                     | 0.54              |
| 25:RA:574:C:N3    | 28:RE:145:LYS:NZ  | 2.55                     | 0.54              |
| 25:RA:947:G:H2'   | 25:RA:948:G:C8    | 2.42                     | 0.54              |
| 28:RE:111:ARG:HG3 | 28:RE:160:TYR:CD2 | 2.43                     | 0.54              |
| 25:RA:2786:U:O2'  | 28:RE:62:PRO:O    | 2.23                     | 0.54              |
| 32:RI:33:ARG:HB3  | 32:RI:35:LEU:HD23 | 1.90                     | 0.54              |
| 37:RR:45:ARG:HA   | 37:RR:95:THR:HG21 | 1.90                     | 0.54              |
| 39:RT:37:GLY:O    | 39:RT:39:ARG:N    | 2.34                     | 0.54              |
| 17:XQ:4:LYS:HE3   | 17:XQ:6:LEU:HD21  | 1.90                     | 0.54              |
| 25:YA:528:A:C2    | 25:YA:2042:A:H2'  | 2.42                     | 0.54              |
| 27:YD:70:TRP:CH2  | 27:YD:150:LYS:HA  | 2.43                     | 0.54              |
| 32:YI:79:ILE:N    | 32:YI:141:LYS:O   | 2.40                     | 0.54              |
| 45:YZ:82:ARG:HG3  | 45:YZ:83:PRO:HD2  | 1.90                     | 0.54              |
| 3:QC:84:ILE:HD11  | 3:QC:88:ARG:HH21  | 1.73                     | 0.53              |
| 19:QS:64:GLU:CG   | 50:R4:55:ARG:HH12 | 2.21                     | 0.53              |
| 50:R4:56:VAL:HA   | 50:R4:60:GLN:HB2  | 1.89                     | 0.53              |
| 25:RA:551:G:H5'   | 25:RA:1220:A:H1'  | 1.89                     | 0.53              |
| 25:RA:1754:C:H5'' | 39:RT:113:LYS:HE3 | 1.90                     | 0.53              |
| 27:RD:44:ASN:HD22 | 27:RD:44:ASN:N    | 2.06                     | 0.53              |
| 45:RZ:76:LEU:HD23 | 45:RZ:76:LEU:H    | 1.73                     | 0.53              |
| 1:XA:1376:U:H2'   | 1:XA:1377:A:C8    | 2.43                     | 0.53              |
| 1:XA:255:G:O6     | 1:XA:266:G:O6     | 2.26                     | 0.53              |
| 1:XA:407:G:H2'    | 1:XA:408:A:H8     | 1.74                     | 0.53              |
| 10:XJ:32:ALA:H    | 10:XJ:78:ASN:HD21 | 1.56                     | 0.53              |
| 25:YA:2015:A:H1'  | 51:Y5:2:ALA:CA    | 2.37                     | 0.53              |
| 27:YD:43:ARG:CB   | 27:YD:54:ARG:HB2  | 2.38                     | 0.53              |
| 25:YA:2680:C:H5'  | 28:YE:189:PRO:HA  | 1.90                     | 0.53              |
| 28:YE:78:LEU:HG   | 28:YE:79:ARG:NE   | 2.23                     | 0.53              |
| 25:YA:2849:U:P    | 39:YT:95:ARG:HH12 | 2.31                     | 0.53              |
| 1:QA:1175:G:H2'   | 1:QA:1176:A:H8    | 1.74                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1318:A:H4'    | 19:QS:11:VAL:HG11  | 1.89                     | 0.53              |
| 2:QB:84:GLU:HB3    | 2:QB:219:VAL:HG21  | 1.89                     | 0.53              |
| 10:QJ:80:LYS:HG2   | 1:XA:1162:C:O2'    | 2.08                     | 0.53              |
| 12:QL:55:VAL:HG12  | 12:QL:69:TYR:HA    | 1.90                     | 0.53              |
| 25:RA:2126:A:N6    | 25:RA:2163:C:O2'   | 2.42                     | 0.53              |
| 25:RA:519:U:H2'    | 25:RA:520:G:H8     | 1.73                     | 0.53              |
| 25:RA:882:G:H1     | 25:RA:894:C:N4     | 2.02                     | 0.53              |
| 25:RA:974(A):C:H4' | 25:RA:975:G:O5'    | 2.08                     | 0.53              |
| 28:RE:21:VAL:CG2   | 28:RE:22:PRO:CB    | 2.58                     | 0.53              |
| 45:RZ:152:ALA:O    | 45:RZ:154:ASP:N    | 2.40                     | 0.53              |
| 1:XA:1327:C:OP2    | 21:XU:12:LYS:NZ    | 2.36                     | 0.53              |
| 2:XB:82:ARG:HA     | 2:XB:92:TYR:CE2    | 2.43                     | 0.53              |
| 3:XC:14:ILE:O      | 3:XC:16:ARG:N      | 2.35                     | 0.53              |
| 11:XK:84:VAL:HG11  | 11:XK:95:ILE:HD11  | 1.90                     | 0.53              |
| 48:Y2:15:LYS:H     | 48:Y2:67:LYS:HE2   | 1.73                     | 0.53              |
| 19:XS:64:GLU:CG    | 50:Y4:55:ARG:HH12  | 2.21                     | 0.53              |
| 25:YA:1341:U:OP2   | 25:YA:1394:U:O2'   | 2.19                     | 0.53              |
| 23:XW:76:A:N6      | 25:YA:2422:A:O4'   | 2.41                     | 0.53              |
| 32:YI:62:LYS:HE3   | 32:YI:134:PRO:HG2  | 1.90                     | 0.53              |
| 33:YN:6:PRO:HG3    | 33:YN:41:ASP:HB2   | 1.89                     | 0.53              |
| 1:QA:1004:A:P      | 1:QA:1025:U:H3     | 2.30                     | 0.53              |
| 35:RP:61:ARG:HD2   | 54:R8:13:ARG:HD2   | 1.90                     | 0.53              |
| 25:RA:1149:G:H2'   | 25:RA:1150:C:C6    | 2.43                     | 0.53              |
| 25:RA:2844:G:H3'   | 25:RA:2845:G:H8    | 1.74                     | 0.53              |
| 29:RF:32:LEU:O     | 29:RF:36:VAL:HG23  | 2.09                     | 0.53              |
| 31:RH:149:ARG:HE   | 31:RH:154:PRO:HG2  | 1.72                     | 0.53              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:HD21 | 1.90                     | 0.53              |
| 39:RT:33:LYS:HD2   | 39:RT:82:LEU:HA    | 1.89                     | 0.53              |
| 45:RZ:58:VAL:O     | 45:RZ:60:GLU:N     | 2.39                     | 0.53              |
| 1:XA:131:C:O2'     | 1:XA:262:A:N3      | 2.35                     | 0.53              |
| 2:XB:162:ILE:O     | 2:XB:185:ILE:HG12  | 2.08                     | 0.53              |
| 10:XJ:4:ILE:HG12   | 10:XJ:100:THR:HG22 | 1.89                     | 0.53              |
| 25:YA:1641:A:H2'   | 25:YA:1642:G:O4'   | 2.08                     | 0.53              |
| 27:YD:244:ARG:HB2  | 27:YD:245:PRO:HD2  | 1.90                     | 0.53              |
| 33:YN:30:ILE:HG23  | 33:YN:52:VAL:HG11  | 1.91                     | 0.53              |
| 35:YP:62:LEU:HB2   | 54:Y8:30:ARG:HH11  | 1.71                     | 0.53              |
| 35:YP:88:LEU:HD12  | 35:YP:95:VAL:HG11  | 1.90                     | 0.53              |
| 41:YV:66:ARG:NH1   | 41:YV:88:ARG:HD3   | 2.23                     | 0.53              |
| 1:QA:1367:C:H4'    | 10:QJ:48:THR:HG21  | 1.90                     | 0.53              |
| 3:QC:35:GLU:HG2    | 3:QC:59:ARG:NH2    | 2.23                     | 0.53              |
| 25:RA:1419:A:H61   | 25:RA:1494:A:H61   | 1.55                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1411:C:N4   | 25:RA:1591:G:H1    | 2.04                     | 0.53              |
| 36:RQ:32:TYR:CE1  | 36:RQ:133:ARG:HG3  | 2.43                     | 0.53              |
| 41:RV:99:ILE:O    | 41:RV:101:GLY:N    | 2.41                     | 0.53              |
| 45:RZ:166:SER:H   | 45:RZ:167:PRO:HA   | 1.74                     | 0.53              |
| 9:XI:111:ARG:NE   | 9:XI:112:LYS:O     | 2.38                     | 0.53              |
| 19:XS:36:ARG:NH1  | 19:XS:52:TYR:O     | 2.42                     | 0.53              |
| 22:XV:28:C:H2'    | 22:XV:29:G:H8      | 1.72                     | 0.53              |
| 25:YA:2286:A:H4'  | 25:YA:2287:A:O4'   | 2.09                     | 0.53              |
| 25:YA:2304:G:H22  | 25:YA:2312:U:H3    | 1.57                     | 0.53              |
| 27:YD:30:GLU:HG3  | 27:YD:63:ARG:HH21  | 1.72                     | 0.53              |
| 38:YS:58:LEU:O    | 38:YS:58:LEU:HD23  | 2.08                     | 0.53              |
| 39:YT:112:ARG:NE  | 39:YT:112:ARG:O    | 2.39                     | 0.53              |
| 39:YT:51:ARG:CG   | 39:YT:98:LYS:HG3   | 2.38                     | 0.53              |
| 1:QA:957:U:H4'    | 19:QS:79:THR:HB    | 1.89                     | 0.53              |
| 4:QD:78:LEU:HD22  | 4:QD:96:LEU:HB3    | 1.89                     | 0.53              |
| 8:QH:51:VAL:HG11  | 8:QH:60:ARG:HG3    | 1.90                     | 0.53              |
| 1:QA:1128:C:H4'   | 9:QI:16:ARG:HH12   | 1.74                     | 0.53              |
| 51:R5:58:LEU:C    | 51:R5:60:VAL:N     | 2.62                     | 0.53              |
| 25:RA:49:A:C8     | 25:RA:120:U:C5     | 2.97                     | 0.53              |
| 34:RO:2:ILE:HD13  | 34:RO:8:LEU:HD11   | 1.90                     | 0.53              |
| 2:XB:60:ASP:O     | 2:XB:64:ARG:HG2    | 2.09                     | 0.53              |
| 51:Y5:40:LYS:NZ   | 51:Y5:46:CYS:SG    | 2.81                     | 0.53              |
| 25:YA:1826:G:H4'  | 27:YD:242:ARG:CZ   | 2.39                     | 0.53              |
| 25:YA:2114:A:N6   | 25:YA:2119:A:N7    | 2.56                     | 0.53              |
| 36:YQ:12:GLN:HG2  | 36:YQ:73:PRO:HD2   | 1.90                     | 0.53              |
| 48:R2:65:ASN:HB3  | 48:R2:69:ARG:NH2   | 2.24                     | 0.53              |
| 45:RZ:5:LEU:HD11  | 45:RZ:39:VAL:HB    | 1.91                     | 0.53              |
| 8:XH:121:ASP:HB2  | 8:XH:125:ARG:NH2   | 2.24                     | 0.53              |
| 55:Y9:27:CYS:SG   | 55:Y9:28:GLU:N     | 2.82                     | 0.53              |
| 25:YA:673:C:OP1   | 29:YF:54:ARG:NH1   | 2.37                     | 0.53              |
| 27:YD:206:LEU:O   | 27:YD:211:ARG:HD3  | 2.09                     | 0.53              |
| 32:YI:93:THR:HG22 | 32:YI:119:PRO:HB3  | 1.91                     | 0.53              |
| 39:YT:105:LEU:O   | 39:YT:107:ASP:N    | 2.42                     | 0.53              |
| 1:QA:1014:A:H4'   | 19:QS:14:HIS:CD2   | 2.44                     | 0.53              |
| 1:QA:51:A:N7      | 1:QA:114:U:O2'     | 2.40                     | 0.53              |
| 1:QA:673:G:H2'    | 1:QA:674:G:C8      | 2.43                     | 0.53              |
| 9:QI:71:SER:HA    | 9:QI:74:ILE:HD12   | 1.90                     | 0.53              |
| 25:RA:1798:U:C5'  | 27:RD:259:THR:HG22 | 2.38                     | 0.53              |
| 25:RA:1799:G:H4'  | 25:RA:1800:C:O5'   | 2.08                     | 0.53              |
| 1:XA:17:U:H2'     | 1:XA:18:C:C6       | 2.44                     | 0.53              |
| 20:XT:47:GLY:O    | 20:XT:49:ALA:N     | 2.41                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:XT:95:ALA:O    | 20:XT:97:ALA:N     | 2.42                     | 0.53              |
| 25:YA:28:A:N6     | 25:YA:512:G:H1'    | 2.23                     | 0.53              |
| 25:YA:862:G:H2'   | 25:YA:863:A:O4'    | 2.08                     | 0.53              |
| 33:YN:13:TRP:O    | 33:YN:135:PRO:HD2  | 2.08                     | 0.53              |
| 33:YN:96:GLU:HG2  | 33:YN:97:ARG:N     | 2.23                     | 0.53              |
| 35:YP:92:GLU:HA   | 35:YP:123:LEU:HD23 | 1.89                     | 0.53              |
| 39:YT:16:ARG:HE   | 39:YT:19:LEU:HD21  | 1.73                     | 0.53              |
| 40:YU:102:GLU:OE1 | 41:YV:13:ARG:NH2   | 2.41                     | 0.53              |
| 1:QA:1263:C:N4    | 1:QA:1272:G:H1     | 2.07                     | 0.53              |
| 1:QA:411:A:C5     | 1:QA:413:G:H1'     | 2.44                     | 0.53              |
| 4:QD:194:LEU:HD12 | 4:QD:195:ALA:H     | 1.73                     | 0.53              |
| 6:QF:10:LEU:HD13  | 6:QF:61:LEU:HD13   | 1.90                     | 0.53              |
| 1:QA:1310:G:OP1   | 13:QM:77:ASN:ND2   | 2.42                     | 0.53              |
| 48:R2:10:LEU:O    | 48:R2:13:ALA:N     | 2.40                     | 0.53              |
| 25:RA:1861:G:H1   | 25:RA:1881:C:H42   | 1.54                     | 0.53              |
| 28:RE:203:LYS:HE3 | 28:RE:204:ALA:HB2  | 1.90                     | 0.53              |
| 29:RF:135:LYS:HB3 | 29:RF:138:GLU:HG3  | 1.90                     | 0.53              |
| 32:RI:88:ILE:O    | 32:RI:121:LYS:NZ   | 2.40                     | 0.53              |
| 35:RP:113:LYS:HG2 | 35:RP:115:LEU:HD23 | 1.90                     | 0.53              |
| 44:RY:98:VAL:HG13 | 44:RY:99:CYS:SG    | 2.48                     | 0.53              |
| 25:YA:1790:C:H5"  | 25:YA:1791:A:OP1   | 2.08                     | 0.53              |
| 25:YA:2496:C:P    | 36:YQ:81:VAL:HG12  | 2.48                     | 0.53              |
| 25:YA:918:A:N3    | 26:YB:80:U:O2'     | 2.38                     | 0.53              |
| 1:QA:1095:U:P     | 1:QA:1108:G:H1     | 2.31                     | 0.53              |
| 1:QA:259:G:H1     | 1:QA:267:C:N4      | 2.07                     | 0.53              |
| 15:QO:6:GLU:OE2   | 15:QO:6:GLU:N      | 2.35                     | 0.53              |
| 25:RA:1050:A:H2'  | 25:RA:1051:G:O4'   | 2.09                     | 0.53              |
| 25:RA:1358:G:N1   | 25:RA:1372:U:OP2   | 2.25                     | 0.53              |
| 25:RA:2505:G:P    | 56:Z7:1:T17:H47    | 2.49                     | 0.53              |
| 27:RD:206:LEU:O   | 27:RD:211:ARG:NH1  | 2.38                     | 0.53              |
| 28:RE:1:MET:N     | 28:RE:83:ASP:O     | 2.41                     | 0.53              |
| 29:RF:157:VAL:HB  | 29:RF:194:MET:HB3  | 1.91                     | 0.53              |
| 1:XA:486:U:H2'    | 1:XA:487:A:C8      | 2.44                     | 0.53              |
| 12:XL:7:ILE:HD13  | 12:XL:10:LEU:HD12  | 1.90                     | 0.53              |
| 6:XF:97:PHE:CD1   | 18:XR:31:LEU:HD21  | 2.43                     | 0.53              |
| 30:YG:179:PRO:HG3 | 50:Y4:38:LYS:NZ    | 2.24                     | 0.53              |
| 52:Y6:26:ASN:ND2  | 52:Y6:35:GLU:OE2   | 2.42                     | 0.53              |
| 25:YA:2154:G:H2'  | 25:YA:2155:G:H8    | 1.73                     | 0.53              |
| 25:YA:27:G:N2     | 25:YA:512:G:H2'    | 2.24                     | 0.53              |
| 27:YD:85:ASP:OD2  | 27:YD:88:ARG:HD2   | 2.08                     | 0.53              |
| 25:YA:2392:A:C8   | 35:YP:60:MET:HG2   | 2.44                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:10:ARG:O     | 38:YS:12:PHE:N    | 2.42                     | 0.53              |
| 1:QA:1105:A:H2'    | 1:QA:1106:G:H8    | 1.74                     | 0.53              |
| 47:R1:80:LEU:HD23  | 47:R1:80:LEU:H    | 1.74                     | 0.53              |
| 25:RA:1165:U:H2'   | 25:RA:1166:C:C6   | 2.44                     | 0.53              |
| 28:RE:21:VAL:CB    | 28:RE:22:PRO:CA   | 2.87                     | 0.53              |
| 25:RA:2482:G:O6    | 36:RQ:124:LYS:NZ  | 2.42                     | 0.53              |
| 42:RW:110:LYS:HG3  | 42:RW:111:HIS:ND1 | 2.23                     | 0.53              |
| 1:XA:1218:C:H2'    | 1:XA:1219:U:C6    | 2.44                     | 0.53              |
| 1:XA:1314:C:OP2    | 19:XS:4:SER:OG    | 2.26                     | 0.53              |
| 1:XA:390:C:H2'     | 1:XA:391:G:C8     | 2.43                     | 0.53              |
| 1:XA:410:G:H2'     | 1:XA:429:U:C5     | 2.45                     | 0.53              |
| 18:XR:25:THR:HB    | 18:XR:26:LEU:HD23 | 1.91                     | 0.53              |
| 19:XS:31:ILE:HG23  | 19:XS:49:ILE:HA   | 1.91                     | 0.53              |
| 31:YH:149:ARG:NH1  | 31:YH:167:GLU:OE1 | 2.42                     | 0.53              |
| 25:YA:996:A:OP2    | 40:YU:92:ARG:NH2  | 2.42                     | 0.53              |
| 1:QA:1189:C:OP1    | 10:QJ:51:ARG:NH2  | 2.41                     | 0.52              |
| 1:QA:346:G:H1'     | 1:QA:347:G:H5'    | 1.90                     | 0.52              |
| 13:QM:66:LEU:HA    | 13:QM:70:LEU:HB2  | 1.91                     | 0.52              |
| 31:RH:10:PRO:HD2   | 31:RH:50:VAL:HG13 | 1.89                     | 0.52              |
| 32:RI:144:VAL:HG22 | 32:RI:145:VAL:H   | 1.73                     | 0.52              |
| 2:XB:44:LEU:HD12   | 2:XB:44:LEU:H     | 1.74                     | 0.52              |
| 23:XW:50:U:H3      | 23:XW:64:A:H2     | 1.54                     | 0.52              |
| 25:YA:1209:G:H21   | 25:YA:1210:A:H62  | 1.56                     | 0.52              |
| 25:YA:2062:A:H1'   | 56:Z8:7:LYS:HB2   | 1.91                     | 0.52              |
| 25:YA:287:C:H2'    | 25:YA:288:C:C6    | 2.43                     | 0.52              |
| 25:YA:605:C:O2     | 25:YA:657:U:O2'   | 2.27                     | 0.52              |
| 4:QD:98:GLU:OE2    | 4:QD:107:ARG:NE   | 2.43                     | 0.52              |
| 1:QA:1316:G:H5''   | 14:QN:17:LYS:HE3  | 1.91                     | 0.52              |
| 19:QS:44:MET:O     | 19:QS:46:GLY:N    | 2.40                     | 0.52              |
| 25:RA:2022:U:OP2   | 51:R5:15:ARG:NH2  | 2.42                     | 0.52              |
| 25:RA:2503:A:O2'   | 25:RA:2505:G:OP2  | 2.24                     | 0.52              |
| 25:RA:2815:C:H5'   | 51:R5:29:THR:HG21 | 1.91                     | 0.52              |
| 25:RA:347:A:H2'    | 25:RA:348:G:H8    | 1.73                     | 0.52              |
| 29:RF:134:GLY:HA3  | 29:RF:165:ARG:NH1 | 2.25                     | 0.52              |
| 31:RH:46:GLU:OE2   | 31:RH:51:ARG:NH1  | 2.42                     | 0.52              |
| 6:XF:97:PHE:O      | 18:XR:30:ASP:OD1  | 2.27                     | 0.52              |
| 7:XG:15:ASP:HB3    | 7:XG:19:GLY:H     | 1.74                     | 0.52              |
| 25:YA:1359:A:N6    | 25:YA:1373:A:C5   | 2.77                     | 0.52              |
| 27:YD:132:PRO:HD3  | 27:YD:190:TYR:CZ  | 2.44                     | 0.52              |
| 44:YY:35:TYR:CE2   | 44:YY:69:ALA:HB3  | 2.44                     | 0.52              |
| 1:QA:1422:G:H5''   | 34:RO:48:PRO:HB3  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:QG:153:HIS:HE1  | 11:QK:57:THR:HG23  | 1.75                     | 0.52              |
| 25:RA:443:A:H3'   | 29:RF:45:ARG:NH1   | 2.23                     | 0.52              |
| 27:RD:133:LEU:HB3 | 27:RD:173:VAL:HG11 | 1.91                     | 0.52              |
| 30:RG:82:LEU:HA   | 30:RG:86:MET:SD    | 2.48                     | 0.52              |
| 26:RB:52:A:H62    | 38:RS:33:LYS:HG3   | 1.73                     | 0.52              |
| 41:RV:60:GLU:HB2  | 41:RV:97:LYS:HE3   | 1.91                     | 0.52              |
| 1:XA:1191:A:H5''  | 3:XC:4:LYS:HZ2     | 1.74                     | 0.52              |
| 1:XA:67:C:H2'     | 1:XA:68:G:H8       | 1.75                     | 0.52              |
| 3:XC:40:ARG:O     | 3:XC:44:GLU:HB2    | 2.09                     | 0.52              |
| 52:Y6:40:CYS:HB2  | 52:Y6:45:LYS:HD3   | 1.90                     | 0.52              |
| 25:YA:2683:C:OP1  | 39:YT:53:ARG:NH2   | 2.38                     | 0.52              |
| 30:YG:96:ARG:O    | 30:YG:98:ARG:N     | 2.42                     | 0.52              |
| 33:YN:110:GLY:O   | 33:YN:114:ARG:HG3  | 2.09                     | 0.52              |
| 26:YB:104:A:H5'   | 45:YZ:72:ARG:HD3   | 1.90                     | 0.52              |
| 1:QA:690:G:H22    | 11:QK:55:LYS:NZ    | 2.08                     | 0.52              |
| 25:RA:2308:G:O6   | 25:RA:2311:A:N1    | 2.42                     | 0.52              |
| 27:RD:35:LYS:NZ   | 27:RD:64:ILE:O     | 2.41                     | 0.52              |
| 31:RH:86:GLU:HG3  | 31:RH:165:ALA:N    | 2.25                     | 0.52              |
| 32:RI:11:ASN:O    | 32:RI:12:LEU:HB2   | 2.09                     | 0.52              |
| 1:XA:1446:A:H5'   | 39:YT:122:ASP:OD1  | 2.10                     | 0.52              |
| 3:XC:189:ALA:HB3  | 3:XC:196:LEU:HB2   | 1.91                     | 0.52              |
| 20:XT:53:LEU:O    | 20:XT:57:ARG:NH1   | 2.42                     | 0.52              |
| 25:YA:551:G:H5'   | 25:YA:1220:A:H1'   | 1.91                     | 0.52              |
| 25:YA:1426:G:OP2  | 25:YA:1427:A:O2'   | 2.28                     | 0.52              |
| 25:YA:1407:C:N4   | 25:YA:1595:G:H1    | 2.08                     | 0.52              |
| 35:YP:64:LYS:HB2  | 54:Y8:25:MET:HG3   | 1.90                     | 0.52              |
| 1:QA:103:C:P      | 20:QT:17:ARG:HH21  | 2.33                     | 0.52              |
| 1:QA:1128:C:H4'   | 9:QI:16:ARG:HH22   | 1.73                     | 0.52              |
| 51:R5:55:ARG:CG   | 51:R5:55:ARG:HH11  | 2.22                     | 0.52              |
| 25:RA:1357:U:H2'  | 25:RA:1358:G:O4'   | 2.09                     | 0.52              |
| 25:RA:1869:G:H5'  | 25:RA:1870:C:OP2   | 2.09                     | 0.52              |
| 25:RA:2438:U:O3'  | 25:RA:2439:A:H3'   | 2.09                     | 0.52              |
| 25:RA:637:A:O5'   | 35:RP:116:GLY:HA2  | 2.08                     | 0.52              |
| 32:RI:55:ALA:C    | 32:RI:58:LEU:HB3   | 2.30                     | 0.52              |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:HD11   | 1.91                     | 0.52              |
| 37:RR:59:ASP:OD2  | 37:RR:61:HIS:HB3   | 2.08                     | 0.52              |
| 50:Y4:54:GLY:O    | 50:Y4:59:PHE:HB2   | 2.09                     | 0.52              |
| 54:Y8:11:LYS:NZ   | 54:Y8:63:PRO:HG3   | 2.24                     | 0.52              |
| 25:YA:828:U:H4'   | 25:YA:831:G:N1     | 2.24                     | 0.52              |
| 38:YS:6:ALA:O     | 38:YS:10:ARG:HD3   | 2.09                     | 0.52              |
| 2:QB:134:GLU:HA   | 2:QB:137:ARG:HB3   | 1.92                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:R2:4:SER:OG     | 48:R2:5:GLU:OE2   | 2.16                     | 0.52              |
| 25:RA:1311:G:H21   | 25:RA:1603:A:N6   | 2.06                     | 0.52              |
| 25:RA:2693:A:H2'   | 25:RA:2694:G:C8   | 2.44                     | 0.52              |
| 25:RA:345:A:H2'    | 25:RA:347:A:H62   | 1.74                     | 0.52              |
| 27:RD:108:PRO:HB3  | 27:RD:143:HIS:HE1 | 1.73                     | 0.52              |
| 52:Y6:13:CYS:O     | 52:Y6:21:TYR:HA   | 2.09                     | 0.52              |
| 29:YF:24:LEU:HD23  | 29:YF:115:ALA:HA  | 1.91                     | 0.52              |
| 13:XM:11:ARG:NH2   | 30:YG:146:TYR:CD2 | 2.67                     | 0.52              |
| 35:YP:20:GLY:HA2   | 35:YP:27:HIS:O    | 2.10                     | 0.52              |
| 1:QA:1126:U:H5     | 1:QA:1127:G:C4    | 2.27                     | 0.52              |
| 1:QA:662:G:H2'     | 1:QA:663:A:C8     | 2.45                     | 0.52              |
| 8:QH:77:GLU:HG2    | 8:QH:78:GLN:H     | 1.74                     | 0.52              |
| 25:RA:1980:G:H4'   | 25:RA:1981:A:OP2  | 2.09                     | 0.52              |
| 25:RA:2232:U:P     | 47:R1:40:ARG:HH12 | 2.33                     | 0.52              |
| 25:RA:608:A:OP1    | 29:RF:100:THR:OG1 | 2.27                     | 0.52              |
| 25:RA:631:A:OP1    | 35:RP:64:LYS:HE2  | 2.10                     | 0.52              |
| 27:RD:206:LEU:HD22 | 27:RD:211:ARG:HG2 | 1.92                     | 0.52              |
| 1:XA:407:G:H2'     | 1:XA:408:A:C8     | 2.45                     | 0.52              |
| 2:XB:35:GLU:O      | 2:XB:36:ARG:HD3   | 2.10                     | 0.52              |
| 10:XJ:78:ASN:O     | 10:XJ:81:THR:OG1  | 2.25                     | 0.52              |
| 49:Y3:40:THR:HB    | 49:Y3:43:ILE:HG12 | 1.92                     | 0.52              |
| 51:Y5:40:LYS:NZ    | 51:Y5:46:CYS:HB2  | 2.24                     | 0.52              |
| 25:YA:2022:U:O2'   | 25:YA:2617:C:H5'  | 2.08                     | 0.52              |
| 29:YF:63:LYS:HE2   | 29:YF:67:GLN:HB2  | 1.91                     | 0.52              |
| 30:YG:88:ILE:O     | 30:YG:88:ILE:HD13 | 2.09                     | 0.52              |
| 25:YA:958:U:OP2    | 36:YQ:14:ARG:NH1  | 2.42                     | 0.52              |
| 1:QA:971:G:N2      | 1:QA:1363:A:OP2   | 2.28                     | 0.52              |
| 19:QS:42:PRO:HD3   | 50:R4:63:TYR:CE1  | 2.44                     | 0.52              |
| 23:QW:33:U:H2'     | 23:QW:35:A:OP2    | 2.09                     | 0.52              |
| 25:RA:1244:G:H4'   | 35:RP:7:ARG:HB2   | 1.92                     | 0.52              |
| 25:RA:2146:C:H4'   | 25:RA:2147:G:C8   | 2.44                     | 0.52              |
| 25:RA:38:A:H2'     | 25:RA:39:C:C6     | 2.45                     | 0.52              |
| 29:RF:150:GLY:HA2  | 29:RF:172:TRP:CE3 | 2.44                     | 0.52              |
| 14:XN:43:CYS:HA    | 14:XN:46:GLU:HG3  | 1.92                     | 0.52              |
| 16:XP:8:ARG:O      | 16:XP:9:PHE:HD1   | 1.93                     | 0.52              |
| 22:XV:29:G:H1      | 22:XV:41:C:H42    | 1.57                     | 0.52              |
| 25:YA:1316:U:H2'   | 25:YA:1317:A:C8   | 2.44                     | 0.52              |
| 1:QA:401:C:O2'     | 1:QA:621:A:N3     | 2.39                     | 0.52              |
| 11:QK:32:ILE:HG13  | 11:QK:72:ALA:HB2  | 1.92                     | 0.52              |
| 18:QR:32:ARG:HA    | 18:QR:69:THR:HG21 | 1.91                     | 0.52              |
| 47:R1:2:SER:HB2    | 47:R1:4:VAL:HG12  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:QS:9:VAL:HG11  | 50:R4:66:SER:O    | 2.09                     | 0.52              |
| 25:RA:1007:C:H5'' | 33:RN:35:ARG:NH1  | 2.25                     | 0.52              |
| 25:RA:1264:G:H3'  | 25:RA:1265:A:H5'' | 1.90                     | 0.52              |
| 25:RA:1689:A:H2'  | 25:RA:1690:A:C8   | 2.44                     | 0.52              |
| 25:RA:25:U:H5'    | 42:RW:79:GLY:HA2  | 1.91                     | 0.52              |
| 25:RA:2776:A:H4'  | 25:RA:2777:G:O5'  | 2.09                     | 0.52              |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:HD2 | 1.92                     | 0.52              |
| 37:RR:33:ARG:HD3  | 37:RR:113:LEU:HG  | 1.92                     | 0.52              |
| 44:RY:84:ARG:O    | 44:RY:95:LYS:HD3  | 2.09                     | 0.52              |
| 45:RZ:111:VAL:CG2 | 45:RZ:112:ARG:H   | 2.12                     | 0.52              |
| 1:XA:833:U:H3     | 1:XA:853:G:H1     | 1.58                     | 0.52              |
| 5:XE:13:ILE:HD11  | 5:XE:55:VAL:HG22  | 1.91                     | 0.52              |
| 7:XG:78:ARG:HG3   | 7:XG:79:ARG:N     | 2.25                     | 0.52              |
| 47:Y1:83:GLU:HG2  | 47:Y1:84:GLY:N    | 2.24                     | 0.52              |
| 48:Y2:58:ALA:O    | 48:Y2:62:THR:HG23 | 2.10                     | 0.52              |
| 52:Y6:7:ILE:HG13  | 52:Y6:8:LYS:H     | 1.75                     | 0.52              |
| 25:YA:2815:C:H5'  | 51:Y5:29:THR:HG21 | 1.92                     | 0.52              |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:N   | 2.25                     | 0.52              |
| 25:YA:2334:G:H5'  | 38:YS:9:ARG:HG2   | 1.91                     | 0.52              |
| 25:RA:818:G:N1    | 25:RA:1188:U:OP2  | 2.28                     | 0.52              |
| 25:RA:2046:G:H5'  | 51:R5:19:ARG:HB2  | 1.91                     | 0.52              |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:H    | 1.56                     | 0.52              |
| 44:RY:87:LYS:HA   | 44:RY:92:ASN:HB3  | 1.91                     | 0.52              |
| 45:RZ:5:LEU:HD21  | 45:RZ:44:PHE:HA   | 1.92                     | 0.52              |
| 1:XA:115:G:H4'    | 1:XA:116:A:O5'    | 2.09                     | 0.52              |
| 1:XA:335:C:O2'    | 1:XA:1433:A:N3    | 2.39                     | 0.52              |
| 1:XA:1443:G:H5'   | 1:XA:1446:A:OP2   | 2.10                     | 0.52              |
| 2:XB:29:ALA:O     | 2:XB:32:ILE:HG22  | 2.10                     | 0.52              |
| 4:XD:108:LEU:HB3  | 4:XD:110:PHE:CE1  | 2.45                     | 0.52              |
| 19:XS:19:VAL:HG11 | 19:XS:44:MET:HG2  | 1.91                     | 0.52              |
| 25:YA:1071:G:O6   | 25:YA:1091:G:O6   | 2.28                     | 0.52              |
| 25:YA:1533:C:N3   | 25:YA:1538:G:N2   | 2.46                     | 0.52              |
| 25:YA:49:A:C8     | 25:YA:120:U:C5    | 2.98                     | 0.52              |
| 35:YP:62:LEU:N    | 35:YP:62:LEU:CD2  | 2.72                     | 0.52              |
| 1:QA:1151:A:H2'   | 1:QA:1152:A:C8    | 2.45                     | 0.51              |
| 1:QA:359:U:H2'    | 1:QA:360:A:C8     | 2.44                     | 0.51              |
| 20:QT:14:LYS:HA   | 20:QT:17:ARG:HG3  | 1.91                     | 0.51              |
| 25:RA:1543:A:C1'  | 25:RA:1545:A:O4'  | 2.53                     | 0.51              |
| 25:RA:177:G:H3'   | 25:RA:178:G:H8    | 1.74                     | 0.51              |
| 25:RA:1942:C:OP2  | 25:RA:1943:U:O2'  | 2.24                     | 0.51              |
| 25:RA:2123:G:H2'  | 25:RA:2124:G:H8   | 1.74                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:RB:111:U:H2'   | 26:RB:112:G:H8     | 1.75                     | 0.51              |
| 41:RV:34:GLU:O    | 41:RV:36:PRO:HD3   | 2.10                     | 0.51              |
| 25:RA:1598:C:H5'  | 43:RX:36:LYS:HB2   | 1.91                     | 0.51              |
| 26:RB:74:U:H1'    | 45:RZ:34:ASN:HD21  | 1.74                     | 0.51              |
| 1:XA:1256:A:OP2   | 3:XC:26:LYS:NZ     | 2.34                     | 0.51              |
| 3:XC:47:LEU:HD11  | 3:XC:76:VAL:HB     | 1.91                     | 0.51              |
| 4:XD:13:ARG:HD2   | 4:XD:38:TYR:O      | 2.10                     | 0.51              |
| 13:XM:14:ARG:N    | 13:XM:44:ARG:HD3   | 2.20                     | 0.51              |
| 20:XT:26:ASN:HB2  | 20:XT:71:THR:HG23  | 1.92                     | 0.51              |
| 23:XW:18:G:H1     | 23:XW:55:U:H1'     | 1.74                     | 0.51              |
| 25:YA:443:A:H5''  | 25:YA:444:C:OP1    | 2.10                     | 0.51              |
| 27:YD:248:SER:HB3 | 27:YD:252:TRP:CZ2  | 2.43                     | 0.51              |
| 30:YG:77:ILE:HD13 | 30:YG:82:LEU:HD12  | 1.92                     | 0.51              |
| 31:YH:88:LEU:H    | 31:YH:88:LEU:HD22  | 1.75                     | 0.51              |
| 39:YT:88:ILE:HD12 | 39:YT:90:GLN:N     | 2.25                     | 0.51              |
| 25:YA:874:G:H5''  | 45:YZ:175:VAL:HG11 | 1.92                     | 0.51              |
| 1:QA:49:U:O4      | 1:QA:365:U:C4      | 2.63                     | 0.51              |
| 12:QL:54:LYS:HD2  | 12:QL:54:LYS:H     | 1.74                     | 0.51              |
| 23:QW:49:C:H42    | 23:QW:65:G:H1      | 1.58                     | 0.51              |
| 25:RA:1899:G:H21  | 25:RA:1902:C:H41   | 1.57                     | 0.51              |
| 27:RD:12:SER:HB2  | 27:RD:208:LYS:HB3  | 1.92                     | 0.51              |
| 29:RF:150:GLY:HA2 | 29:RF:172:TRP:CD2  | 2.45                     | 0.51              |
| 29:RF:47:GLY:HA3  | 29:RF:95:ARG:O     | 2.10                     | 0.51              |
| 31:RH:86:GLU:H    | 31:RH:86:GLU:CD    | 2.12                     | 0.51              |
| 1:XA:188:U:H2'    | 1:XA:189:U:H5''    | 1.92                     | 0.51              |
| 1:XA:977:A:O2'    | 1:XA:979:C:OP2     | 2.22                     | 0.51              |
| 2:XB:170:GLU:O    | 2:XB:174:VAL:HG23  | 2.11                     | 0.51              |
| 9:XI:70:LYS:O     | 9:XI:74:ILE:HG13   | 2.10                     | 0.51              |
| 12:XL:77:LEU:HD21 | 12:XL:107:ALA:HA   | 1.92                     | 0.51              |
| 54:Y8:51:ALA:N    | 54:Y8:53:PRO:HD2   | 2.24                     | 0.51              |
| 25:YA:771:G:OP1   | 53:Y7:14:LYS:HE3   | 2.10                     | 0.51              |
| 27:YD:250:TRP:HE3 | 27:YD:252:TRP:HE1  | 1.58                     | 0.51              |
| 31:YH:26:VAL:HG13 | 31:YH:27:LYS:H     | 1.76                     | 0.51              |
| 40:YU:107:ALA:O   | 40:YU:110:VAL:HB   | 2.10                     | 0.51              |
| 42:YW:40:ASN:O    | 42:YW:41:LYS:HG2   | 2.10                     | 0.51              |
| 4:QD:12:CYS:HA    | 4:QD:19:LEU:HD23   | 1.92                     | 0.51              |
| 5:QE:91:LEU:HD12  | 5:QE:120:THR:HG22  | 1.93                     | 0.51              |
| 11:QK:96:ARG:HA   | 11:QK:99:GLN:HE21  | 1.76                     | 0.51              |
| 3:QC:37:GLN:NE2   | 14:QN:52:GLN:OE1   | 2.32                     | 0.51              |
| 25:RA:2126:A:H2   | 25:RA:2162:G:H21   | 1.59                     | 0.51              |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:HG13 | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:RT:111:ARG:C    | 39:RT:113:LYS:H    | 2.12                     | 0.51              |
| 43:RX:35:THR:HG23  | 43:RX:38:GLU:HG2   | 1.92                     | 0.51              |
| 44:RY:74:PRO:O     | 44:RY:80:GLY:HA2   | 2.10                     | 0.51              |
| 1:XA:1376:U:H2'    | 1:XA:1377:A:H8     | 1.74                     | 0.51              |
| 1:XA:643:C:H2'     | 1:XA:644:G:H8      | 1.75                     | 0.51              |
| 17:XQ:100:LYS:O    | 17:XQ:101:ARG:NE   | 2.42                     | 0.51              |
| 20:XT:89:ARG:HH21  | 20:XT:104:LEU:HD11 | 1.76                     | 0.51              |
| 47:Y1:70:VAL:O     | 47:Y1:74:VAL:HG23  | 2.10                     | 0.51              |
| 51:Y5:56:LYS:HD3   | 51:Y5:58:LEU:HD23  | 1.90                     | 0.51              |
| 27:YD:148:GLU:HB2  | 27:YD:151:LYS:HD2  | 1.92                     | 0.51              |
| 25:YA:2224:G:OP1   | 27:YD:268:ARG:HD3  | 2.11                     | 0.51              |
| 32:YI:110:ASP:N    | 32:YI:130:TYR:OH   | 2.43                     | 0.51              |
| 33:YN:38:HIS:O     | 40:YU:67:ALA:HB1   | 2.10                     | 0.51              |
| 37:YR:83:ILE:HG22  | 37:YR:87:TYR:HE2   | 1.76                     | 0.51              |
| 41:YV:25:LEU:H     | 41:YV:92:THR:HG21  | 1.74                     | 0.51              |
| 45:YZ:124:ILE:HG22 | 45:YZ:126:VAL:HG13 | 1.92                     | 0.51              |
| 1:QA:1305:G:H1'    | 1:QA:1332:A:N6     | 2.25                     | 0.51              |
| 1:QA:368:U:P       | 32:YI:91:SER:HG    | 2.34                     | 0.51              |
| 22:QV:23:C:H2'     | 22:QV:24:U:C6      | 2.45                     | 0.51              |
| 25:RA:347:A:H2'    | 25:RA:348:G:C8     | 2.45                     | 0.51              |
| 25:RA:806:C:P      | 35:RP:41:ARG:HH11  | 2.31                     | 0.51              |
| 1:XA:1443:G:H5''   | 1:XA:1446:A:C2     | 2.45                     | 0.51              |
| 1:XA:429:U:H1'     | 1:XA:430:A:H5''    | 1.92                     | 0.51              |
| 2:XB:21:ARG:HB2    | 2:XB:39:ILE:HA     | 1.91                     | 0.51              |
| 23:XW:67:C:H2'     | 23:XW:68:C:C6      | 2.45                     | 0.51              |
| 48:Y2:24:LEU:HD13  | 48:Y2:60:LEU:HD11  | 1.92                     | 0.51              |
| 1:XA:1312:G:OP1    | 50:Y4:58:ARG:NH1   | 2.44                     | 0.51              |
| 51:Y5:42:PRO:HB2   | 51:Y5:43:HIS:ND1   | 2.25                     | 0.51              |
| 25:YA:1972:A:H2'   | 25:YA:1973:G:H8    | 1.74                     | 0.51              |
| 25:YA:2298:A:H2'   | 25:YA:2299:G:O4'   | 2.11                     | 0.51              |
| 25:YA:2469:A:H5''  | 25:YA:2470:G:C8    | 2.46                     | 0.51              |
| 30:YG:16:ARG:O     | 30:YG:20:ILE:HG12  | 2.10                     | 0.51              |
| 25:YA:1093:G:H5'   | 31:YH:170:ARG:NH1  | 2.26                     | 0.51              |
| 32:YI:41:GLU:HG2   | 32:YI:42:SER:N     | 2.24                     | 0.51              |
| 35:YP:96:THR:HG22  | 35:YP:126:VAL:HB   | 1.93                     | 0.51              |
| 25:YA:2250:G:C4    | 36:YQ:82:ARG:HG3   | 2.46                     | 0.51              |
| 41:YV:65:GLY:HA3   | 41:YV:91:TYR:CZ    | 2.46                     | 0.51              |
| 1:QA:539:A:H2'     | 1:QA:540:G:C8      | 2.46                     | 0.51              |
| 1:QA:963:G:H21     | 10:QJ:55:LYS:HE2   | 1.75                     | 0.51              |
| 4:QD:61:LYS:HB2    | 4:QD:203:VAL:HG13  | 1.93                     | 0.51              |
| 10:QJ:31:GLY:HA3   | 10:QJ:78:ASN:ND2   | 2.26                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:947:G:O3'    | 13:QM:109:THR:OG1  | 2.28                     | 0.51              |
| 25:RA:2418:A:OP2  | 54:R8:29:LYS:HE2   | 2.11                     | 0.51              |
| 26:RB:50:G:H5'    | 38:RS:61:ASN:ND2   | 2.26                     | 0.51              |
| 40:RU:90:VAL:HG22 | 41:RV:39:LEU:HB3   | 1.93                     | 0.51              |
| 1:XA:1130:A:N6    | 1:XA:1131:G:O6     | 2.43                     | 0.51              |
| 1:XA:1151:A:H2'   | 1:XA:1152:A:H8     | 1.75                     | 0.51              |
| 5:XE:102:ALA:HB1  | 5:XE:106:PRO:HG2   | 1.93                     | 0.51              |
| 9:XI:11:LYS:H     | 9:XI:104:ARG:HH21  | 1.58                     | 0.51              |
| 48:Y2:65:ASN:HB3  | 48:Y2:69:ARG:NH2   | 2.26                     | 0.51              |
| 25:YA:2011:U:OP1  | 42:YW:42:ARG:NH1   | 2.44                     | 0.51              |
| 29:YF:127:GLU:OE1 | 29:YF:196:LEU:HB2  | 2.11                     | 0.51              |
| 1:QA:1043:C:H2'   | 1:QA:1044:A:H8     | 1.76                     | 0.51              |
| 1:QA:1326:C:OP1   | 21:QU:17:THR:OG1   | 2.17                     | 0.51              |
| 1:QA:833:U:H3     | 1:QA:853:G:H1      | 1.56                     | 0.51              |
| 25:RA:391:G:O2'   | 25:RA:410:G:OP1    | 2.26                     | 0.51              |
| 28:RE:23:VAL:HA   | 28:RE:184:VAL:O    | 2.11                     | 0.51              |
| 43:RX:59:VAL:HG21 | 43:RX:78:LYS:HE3   | 1.91                     | 0.51              |
| 1:XA:971:G:H22    | 1:XA:1363:A:H5'    | 1.75                     | 0.51              |
| 1:XA:812:C:H4'    | 1:XA:813:U:H5'     | 1.93                     | 0.51              |
| 19:XS:15:LEU:O    | 19:XS:19:VAL:N     | 2.36                     | 0.51              |
| 51:Y5:45:VAL:HG11 | 51:Y5:57:VAL:HG12  | 1.93                     | 0.51              |
| 28:YE:62:PRO:O    | 28:YE:64:LYS:N     | 2.43                     | 0.51              |
| 25:YA:2377:A:O2'  | 38:YS:111:GLU:O    | 2.18                     | 0.51              |
| 38:YS:11:LYS:HB2  | 38:YS:91:PRO:HB3   | 1.93                     | 0.51              |
| 39:YT:109:GLU:O   | 39:YT:113:LYS:HB2  | 2.11                     | 0.51              |
| 40:YU:47:TYR:HA   | 40:YU:50:ARG:NH2   | 2.26                     | 0.51              |
| 42:YW:106:ILE:O   | 42:YW:106:ILE:HG12 | 2.07                     | 0.51              |
| 1:QA:390:C:H2'    | 1:QA:391:G:C8      | 2.46                     | 0.51              |
| 1:QA:718:G:H5'    | 11:QK:117:ASN:ND2  | 2.24                     | 0.51              |
| 11:QK:33:THR:HG22 | 11:QK:39:PRO:HA    | 1.92                     | 0.51              |
| 21:QU:6:ARG:HE    | 21:QU:15:ARG:HH21  | 1.58                     | 0.51              |
| 25:RA:2121:G:O6   | 25:RA:2176:A:N6    | 2.43                     | 0.51              |
| 26:RB:15:A:H5'    | 26:RB:16:G:C8      | 2.45                     | 0.51              |
| 28:RE:134:ILE:HA  | 28:RE:137:HIS:CD2  | 2.45                     | 0.51              |
| 29:RF:185:ASP:HA  | 29:RF:188:ARG:HD3  | 1.93                     | 0.51              |
| 32:RI:52:ARG:CB   | 32:RI:56:LYS:HB2   | 2.32                     | 0.51              |
| 1:XA:1226:C:H4'   | 1:XA:1227:A:OP1    | 2.11                     | 0.51              |
| 1:XA:337:C:H2'    | 1:XA:338:A:C8      | 2.46                     | 0.51              |
| 1:XA:484:G:H4'    | 1:XA:485:G:O5'     | 2.11                     | 0.51              |
| 1:XA:719:C:H1'    | 18:XR:49:LYS:HB3   | 1.91                     | 0.51              |
| 7:XG:155:ARG:NH2  | 7:XG:155:ARG:O     | 2.43                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:XK:41:THR:HG21 | 11:XK:71:LYS:HB3   | 1.93                     | 0.51              |
| 25:YA:1820:U:C2   | 27:YD:202:LYS:HB3  | 2.46                     | 0.51              |
| 25:YA:414:C:O2    | 25:YA:1864:U:O2'   | 2.25                     | 0.51              |
| 26:YB:44:G:H5''   | 26:YB:45:A:OP1     | 2.11                     | 0.51              |
| 27:YD:35:LYS:NZ   | 27:YD:104:TYR:HB2  | 2.26                     | 0.51              |
| 31:YH:6:ARG:NE    | 31:YH:54:ARG:HH12  | 2.09                     | 0.51              |
| 32:YI:11:ASN:O    | 32:YI:12:LEU:HB2   | 2.11                     | 0.51              |
| 40:YU:92:ARG:NH1  | 41:YV:11:GLN:O     | 2.44                     | 0.51              |
| 25:YA:142:G:H1'   | 43:YX:37:THR:HG21  | 1.93                     | 0.51              |
| 36:YQ:134:ARG:NH2 | 45:YZ:122:ARG:HH21 | 1.98                     | 0.51              |
| 12:QL:69:TYR:CG   | 12:QL:90:VAL:HG21  | 2.46                     | 0.51              |
| 25:RA:1403:C:H5'' | 25:RA:1471:A:H1'   | 1.92                     | 0.51              |
| 25:RA:1543:A:H2   | 25:RA:1545:A:C5    | 2.29                     | 0.51              |
| 25:RA:67:U:H3     | 25:RA:74:A:H2      | 1.54                     | 0.51              |
| 26:RB:16:G:H1     | 26:RB:68:C:H42     | 1.59                     | 0.51              |
| 29:RF:20:LEU:HD23 | 29:RF:125:LEU:HD12 | 1.93                     | 0.51              |
| 30:RG:88:ILE:HD13 | 30:RG:88:ILE:O     | 2.10                     | 0.51              |
| 31:RH:127:GLU:CB  | 31:RH:130:ARG:HB3  | 2.40                     | 0.51              |
| 38:RS:56:LEU:HD23 | 38:RS:58:LEU:HD22  | 1.92                     | 0.51              |
| 39:RT:28:VAL:HG23 | 39:RT:88:ILE:HA    | 1.92                     | 0.51              |
| 1:XA:606:G:H1     | 1:XA:631:G:H5''    | 1.76                     | 0.51              |
| 6:XF:86:ARG:O     | 6:XF:87:ARG:HG2    | 2.11                     | 0.51              |
| 20:XT:10:LEU:O    | 20:XT:13:LEU:HG    | 2.11                     | 0.51              |
| 49:Y3:43:ILE:O    | 49:Y3:47:VAL:HG23  | 2.10                     | 0.51              |
| 25:YA:16:G:H5''   | 51:Y5:17:ASP:HB2   | 1.92                     | 0.51              |
| 25:YA:2850:A:N7   | 25:YA:2868:A:O2'   | 2.37                     | 0.51              |
| 37:YR:104:ARG:HD3 | 37:YR:111:LEU:HD21 | 1.92                     | 0.51              |
| 6:QF:69:GLU:H     | 6:QF:69:GLU:CD     | 2.15                     | 0.51              |
| 8:QH:20:TYR:HE2   | 8:QH:75:ARG:HD2    | 1.76                     | 0.51              |
| 53:R7:9:ARG:HH21  | 53:R7:48:LYS:HB2   | 1.76                     | 0.51              |
| 32:RI:55:ALA:HA   | 32:RI:58:LEU:HB3   | 1.93                     | 0.51              |
| 42:RW:67:ASP:OD1  | 42:RW:67:ASP:N     | 2.33                     | 0.51              |
| 43:RX:40:LYS:HG3  | 43:RX:51:VAL:HB    | 1.92                     | 0.51              |
| 1:XA:359:U:H2'    | 1:XA:360:A:C8      | 2.46                     | 0.51              |
| 6:XF:4:TYR:HD1    | 6:XF:92:LYS:HA     | 1.76                     | 0.51              |
| 15:XO:33:THR:HG21 | 15:XO:85:LEU:HD22  | 1.93                     | 0.51              |
| 19:XS:26:GLY:O    | 19:XS:28:LYS:N     | 2.43                     | 0.51              |
| 22:XV:15:C:O2'    | 22:XV:61:C:OP1     | 2.28                     | 0.51              |
| 13:XM:62:ASN:HA   | 50:Y4:49:PHE:CE2   | 2.45                     | 0.51              |
| 54:Y8:23:VAL:CG1  | 54:Y8:46:ARG:HD3   | 2.40                     | 0.51              |
| 25:YA:2115:G:N2   | 25:YA:2165:G:N7    | 2.49                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2347:C:H2'   | 25:YA:2348:U:C6    | 2.46                     | 0.51              |
| 31:YH:89:ILE:HG12  | 31:YH:89:ILE:O     | 2.10                     | 0.51              |
| 36:YQ:2:LEU:H      | 36:YQ:2:LEU:HD23   | 1.76                     | 0.51              |
| 44:YY:81:LYS:HG2   | 44:YY:97:ARG:HD3   | 1.93                     | 0.51              |
| 1:QA:1152:A:OP1    | 10:QJ:68:HIS:NE2   | 2.43                     | 0.51              |
| 4:QD:167:GLY:HA2   | 27:YD:135:PHE:HZ   | 1.71                     | 0.51              |
| 1:QA:1147:C:HO2'   | 9:QI:5:TYR:HH      | 1.59                     | 0.51              |
| 12:QL:38:THR:HG23  | 12:QL:57:LYS:HB3   | 1.93                     | 0.51              |
| 25:RA:1009:A:OP2   | 25:RA:1010:A:OP2   | 2.28                     | 0.51              |
| 25:RA:1203:G:O6    | 25:RA:1204:A:N6    | 2.44                     | 0.51              |
| 25:RA:693:C:O2'    | 25:RA:1353:A:N3    | 2.41                     | 0.51              |
| 25:RA:2443:C:H2'   | 25:RA:2444:G:C8    | 2.44                     | 0.51              |
| 25:RA:2832:U:H4'   | 25:RA:2833:G:H5''  | 1.92                     | 0.51              |
| 36:RQ:20:ALA:HB3   | 45:RZ:79:ARG:NH1   | 2.26                     | 0.51              |
| 1:XA:1404:C:H2'    | 1:XA:1405:G:C8     | 2.46                     | 0.51              |
| 1:XA:1104:G:O5'    | 2:XB:111:ARG:HD2   | 2.11                     | 0.51              |
| 1:XA:1492:A:OP1    | 12:XL:47:LYS:N     | 2.44                     | 0.51              |
| 22:XV:8:G:O2'      | 22:XV:9:G:N7       | 2.43                     | 0.51              |
| 54:Y8:58:ILE:HA    | 54:Y8:61:LEU:HD21  | 1.92                     | 0.51              |
| 25:YA:1050:A:H8    | 25:YA:2751:G:HO2'  | 1.58                     | 0.51              |
| 25:YA:639:U:H2'    | 25:YA:640:C:C6     | 2.46                     | 0.51              |
| 25:YA:625:G:O6     | 35:YP:107:LYS:HE2  | 2.11                     | 0.51              |
| 25:YA:1649:G:O2'   | 37:YR:107:ASP:OD2  | 2.20                     | 0.51              |
| 1:QA:446:G:H1      | 1:QA:488:C:H42     | 1.59                     | 0.50              |
| 1:QA:7:G:H5'       | 1:QA:298:A:O4'     | 2.11                     | 0.50              |
| 9:QI:8:GLY:HA2     | 9:QI:79:LEU:HD12   | 1.92                     | 0.50              |
| 16:QP:3:LYS:HG3    | 16:QP:24:ALA:HB2   | 1.92                     | 0.50              |
| 25:RA:111:A:H4'    | 48:R2:69:ARG:NH2   | 2.26                     | 0.50              |
| 51:R5:3:LYS:HA     | 51:R5:3:LYS:NZ     | 2.27                     | 0.50              |
| 51:R5:35:GLU:HB2   | 51:R5:49:CYS:SG    | 2.51                     | 0.50              |
| 25:RA:1443:G:H1    | 25:RA:1548:C:N4    | 2.04                     | 0.50              |
| 25:RA:458:G:O2'    | 25:RA:469:G:O6     | 2.19                     | 0.50              |
| 28:RE:176:ILE:HG23 | 28:RE:178:GLU:OE2  | 2.11                     | 0.50              |
| 35:RP:14:LYS:HD3   | 35:RP:14:LYS:O     | 2.11                     | 0.50              |
| 39:RT:118:ARG:HH21 | 39:RT:121:ILE:HG21 | 1.76                     | 0.50              |
| 39:RT:19:LEU:HD22  | 39:RT:86:ILE:HG22  | 1.93                     | 0.50              |
| 44:RY:97:ARG:HH21  | 44:RY:98:VAL:HB    | 1.77                     | 0.50              |
| 1:XA:1123:A:H4'    | 10:XJ:36:GLY:HA3   | 1.93                     | 0.50              |
| 1:XA:812:C:H1'     | 1:XA:813:U:OP2     | 2.10                     | 0.50              |
| 2:XB:9:GLU:HB3     | 2:XB:48:MET:SD     | 2.50                     | 0.50              |
| 4:XD:78:LEU:HD22   | 4:XD:96:LEU:HB3    | 1.92                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1210:A:H5''  | 25:YA:1212:G:O4'  | 2.11                     | 0.50              |
| 36:YQ:66:ILE:O     | 36:YQ:104:PHE:N   | 2.39                     | 0.50              |
| 28:YE:111:ARG:HA   | 37:YR:1:MET:CG    | 2.40                     | 0.50              |
| 42:YW:57:ASN:O     | 42:YW:61:ASN:HB2  | 2.10                     | 0.50              |
| 9:QI:118:LYS:O     | 9:QI:120:ARG:N    | 2.40                     | 0.50              |
| 10:QJ:22:LYS:HZ2   | 10:QJ:23:ILE:HA   | 1.77                     | 0.50              |
| 13:QM:33:ALA:HA    | 13:QM:59:TYR:HE2  | 1.76                     | 0.50              |
| 25:RA:1363:C:O2'   | 25:RA:1809:A:N3   | 2.37                     | 0.50              |
| 25:RA:94:G:H21     | 48:R2:47:ASN:HD22 | 1.59                     | 0.50              |
| 33:RN:46:VAL:HG13  | 33:RN:48:MET:HG3  | 1.93                     | 0.50              |
| 36:RQ:17:LEU:HD23  | 36:RQ:96:VAL:HG23 | 1.92                     | 0.50              |
| 3:XC:138:VAL:HG22  | 3:XC:151:VAL:HG23 | 1.93                     | 0.50              |
| 50:Y4:10:VAL:HG22  | 50:Y4:11:PRO:HD2  | 1.93                     | 0.50              |
| 1:QA:752:G:H1'     | 1:QA:754:C:H41    | 1.75                     | 0.50              |
| 13:QM:40:ASN:HD22  | 13:QM:43:THR:HG23 | 1.76                     | 0.50              |
| 25:RA:1427:A:H4'   | 25:RA:1428:C:O5'  | 2.10                     | 0.50              |
| 25:RA:2777:G:OP2   | 25:RA:2781:A:O2'  | 2.23                     | 0.50              |
| 25:RA:620:G:H4'    | 25:RA:621:A:H5''  | 1.94                     | 0.50              |
| 25:RA:259:G:O2'    | 25:RA:621:A:O2'   | 2.24                     | 0.50              |
| 31:RH:132:ARG:HH11 | 31:RH:132:ARG:HB2 | 1.76                     | 0.50              |
| 2:XB:80:ILE:HD11   | 2:XB:208:ILE:HG23 | 1.93                     | 0.50              |
| 25:YA:2610:C:H4'   | 25:YA:2611:U:OP2  | 2.10                     | 0.50              |
| 13:XM:68:GLY:C     | 30:YG:116:ASP:OD2 | 2.49                     | 0.50              |
| 36:YQ:89:ASN:O     | 36:YQ:91:GLU:N    | 2.44                     | 0.50              |
| 38:YS:30:ARG:HG3   | 38:YS:97:ARG:NH2  | 2.26                     | 0.50              |
| 1:QA:20:U:H2'      | 1:QA:21:G:C8      | 2.46                     | 0.50              |
| 1:QA:362:G:N2      | 1:QA:365:U:OP2    | 2.44                     | 0.50              |
| 1:QA:963:G:H21     | 10:QJ:55:LYS:CE   | 2.25                     | 0.50              |
| 23:QW:16:U:H3'     | 23:QW:17:C:H5'    | 1.93                     | 0.50              |
| 53:R7:5:TRP:NE1    | 53:R7:7:PRO:HG3   | 2.26                     | 0.50              |
| 28:RE:6:GLY:HA2    | 28:RE:51:PHE:CZ   | 2.46                     | 0.50              |
| 36:RQ:89:ASN:O     | 36:RQ:92:GLY:N    | 2.42                     | 0.50              |
| 1:XA:703:G:H4'     | 1:XA:704:A:O5'    | 2.10                     | 0.50              |
| 2:XB:189:ASP:HB3   | 2:XB:203:GLY:O    | 2.12                     | 0.50              |
| 3:XC:54:ARG:HD3    | 3:XC:56:ASP:OD1   | 2.10                     | 0.50              |
| 19:XS:4:SER:O      | 19:XS:5:LEU:HD13  | 2.11                     | 0.50              |
| 25:YA:910:A:N3     | 25:YA:2264:C:O2'  | 2.39                     | 0.50              |
| 30:YG:5:VAL:HG11   | 30:YG:100:TRP:HB3 | 1.93                     | 0.50              |
| 31:YH:10:PRO:CG    | 31:YH:50:VAL:CG1  | 2.76                     | 0.50              |
| 41:YV:52:VAL:HG23  | 41:YV:55:ALA:H    | 1.76                     | 0.50              |
| 1:QA:1064:G:HO2'   | 1:QA:1065:U:P     | 2.35                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:413:G:H8     | 1:QA:413:G:OP2     | 1.95                     | 0.50              |
| 7:QG:116:ALA:O    | 7:QG:120:ILE:HG12  | 2.11                     | 0.50              |
| 10:QJ:47:PHE:CE1  | 10:QJ:63:PHE:HB2   | 2.47                     | 0.50              |
| 37:RR:33:ARG:NH1  | 51:R5:57:VAL:CG2   | 2.75                     | 0.50              |
| 35:RP:62:LEU:CD2  | 54:R8:25:MET:HB2   | 2.37                     | 0.50              |
| 25:RA:1205:U:C4   | 29:RF:171:PRO:HA   | 2.46                     | 0.50              |
| 25:RA:2789:C:H1'  | 25:RA:2892:A:H2    | 1.75                     | 0.50              |
| 39:RT:111:ARG:O   | 39:RT:113:LYS:N    | 2.42                     | 0.50              |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:N     | 2.09                     | 0.50              |
| 1:XA:280:C:H3'    | 1:XA:281:G:H5'     | 1.94                     | 0.50              |
| 1:XA:677:U:H3     | 1:XA:713:G:H22     | 1.59                     | 0.50              |
| 1:XA:89:U:O2'     | 1:XA:90:C:OP1      | 2.27                     | 0.50              |
| 2:XB:111:ARG:HH21 | 2:XB:114:ARG:HG2   | 1.76                     | 0.50              |
| 19:XS:40:ILE:HG23 | 19:XS:67:VAL:O     | 2.12                     | 0.50              |
| 22:XV:14:G:H22    | 22:XV:48:C:H42     | 1.60                     | 0.50              |
| 25:YA:1061:U:H3'  | 25:YA:1062:G:H5''  | 1.93                     | 0.50              |
| 25:YA:1264:G:H3'  | 25:YA:1265:A:H5''  | 1.94                     | 0.50              |
| 25:YA:470:A:H2'   | 25:YA:471:A:O4'    | 2.11                     | 0.50              |
| 25:YA:747:U:OP2   | 51:Y5:3:LYS:HD2    | 2.12                     | 0.50              |
| 29:YF:167:ALA:HB1 | 29:YF:173:VAL:HG11 | 1.93                     | 0.50              |
| 32:YI:13:GLY:HA3  | 32:YI:17:GLN:OE1   | 2.12                     | 0.50              |
| 1:QA:368:U:OP1    | 32:YI:91:SER:OG    | 2.30                     | 0.50              |
| 34:YO:120:GLU:HG2 | 34:YO:122:LEU:HG   | 1.94                     | 0.50              |
| 35:YP:64:LYS:CB   | 54:Y8:25:MET:HG3   | 2.42                     | 0.50              |
| 9:QI:95:LYS:NZ    | 9:QI:96:LEU:HD13   | 2.26                     | 0.50              |
| 47:R1:62:VAL:HG23 | 47:R1:63:ALA:O     | 2.11                     | 0.50              |
| 25:RA:1140:C:OP1  | 33:RN:23:LEU:HB3   | 2.10                     | 0.50              |
| 25:RA:407:G:H2'   | 25:RA:408:G:C8     | 2.46                     | 0.50              |
| 39:RT:39:ARG:HG2  | 39:RT:40:THR:H     | 1.76                     | 0.50              |
| 45:RZ:91:LEU:HD11 | 45:RZ:96:VAL:HG21  | 1.92                     | 0.50              |
| 1:XA:1241:G:H2'   | 1:XA:1242:C:C6     | 2.46                     | 0.50              |
| 1:XA:1525:G:P     | 11:XK:120:ARG:HH22 | 2.35                     | 0.50              |
| 1:XA:96:G:H2'     | 1:XA:97:U:O4'      | 2.12                     | 0.50              |
| 2:XB:21:ARG:O     | 2:XB:23:ARG:N      | 2.44                     | 0.50              |
| 22:XV:19:G:H5'    | 22:XV:20:U:C5      | 2.46                     | 0.50              |
| 29:YF:65:TRP:O    | 29:YF:67:GLN:N     | 2.43                     | 0.50              |
| 31:YH:84:SER:O    | 31:YH:85:LYS:HB2   | 2.11                     | 0.50              |
| 1:XA:339:C:OP2    | 34:YO:97:ARG:NH1   | 2.45                     | 0.50              |
| 35:YP:36:LYS:HB3  | 35:YP:40:SER:HB3   | 1.94                     | 0.50              |
| 2:QB:231:GLU:HG3  | 2:QB:233:SER:H     | 1.77                     | 0.50              |
| 9:QI:53:VAL:HB    | 9:QI:95:LYS:HE3    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:QM:40:ASN:ND2   | 13:QM:43:THR:HG23  | 2.27                     | 0.50              |
| 54:R8:23:VAL:HG11  | 54:R8:46:ARG:HD3   | 1.92                     | 0.50              |
| 25:RA:1542:G:C3'   | 25:RA:1543:A:C5'   | 2.76                     | 0.50              |
| 25:RA:2277:G:OP2   | 46:R0:10:THR:HG21  | 2.11                     | 0.50              |
| 25:RA:2306:C:H2'   | 25:RA:2307:G:N2    | 2.26                     | 0.50              |
| 25:RA:270(L):U:H2' | 32:RI:50:ARG:HD2   | 1.94                     | 0.50              |
| 25:RA:760:G:H2'    | 25:RA:761:A:O4'    | 2.12                     | 0.50              |
| 29:RF:16:GLY:O     | 29:RF:18:ARG:N     | 2.45                     | 0.50              |
| 32:RI:29:TYR:O     | 32:RI:33:ARG:HB2   | 2.12                     | 0.50              |
| 35:RP:26:GLY:O     | 35:RP:28:GLY:N     | 2.45                     | 0.50              |
| 1:XA:1024:G:OP1    | 1:XA:1024:G:H4'    | 2.12                     | 0.50              |
| 1:XA:582:U:H2'     | 1:XA:583:A:C8      | 2.47                     | 0.50              |
| 1:XA:7:G:H5'       | 1:XA:298:A:O4'     | 2.12                     | 0.50              |
| 2:XB:114:ARG:O     | 2:XB:117:GLU:HB2   | 2.11                     | 0.50              |
| 2:XB:162:ILE:HD11  | 2:XB:184:VAL:HG22  | 1.94                     | 0.50              |
| 4:XD:108:LEU:HD21  | 4:XD:183:GLY:HA3   | 1.93                     | 0.50              |
| 4:XD:112:VAL:HG12  | 4:XD:116:GLN:OE1   | 2.12                     | 0.50              |
| 5:XE:76:ILE:HG13   | 5:XE:93:PRO:HB3    | 1.94                     | 0.50              |
| 11:XK:86:GLY:O     | 11:XK:91:ARG:HD3   | 2.11                     | 0.50              |
| 25:YA:1278:A:H4'   | 37:YR:34:ILE:HD12  | 1.94                     | 0.50              |
| 11:QK:17:GLY:N     | 11:QK:79:SER:O     | 2.44                     | 0.50              |
| 25:RA:1790:C:H5''  | 25:RA:1791:A:OP1   | 2.11                     | 0.50              |
| 25:RA:2103:C:H42   | 25:RA:2186:G:H1    | 1.59                     | 0.50              |
| 25:RA:270(H):C:H42 | 25:RA:270(R):G:H1  | 1.60                     | 0.50              |
| 27:RD:62:TYR:CE2   | 27:RD:64:ILE:HA    | 2.46                     | 0.50              |
| 36:RQ:134:ARG:NH2  | 45:RZ:122:ARG:HD2  | 2.27                     | 0.50              |
| 1:XA:1147:C:HO2'   | 9:XI:5:TYR:HH      | 1.58                     | 0.50              |
| 2:XB:32:ILE:HD11   | 2:XB:40:HIS:HB3    | 1.94                     | 0.50              |
| 52:Y6:47:THR:HG22  | 52:Y6:48:VAL:HG12  | 1.94                     | 0.50              |
| 25:YA:1109:C:O2'   | 25:YA:1110:G:OP1   | 2.30                     | 0.50              |
| 25:YA:2319:G:N7    | 38:YS:3:ARG:HB3    | 2.27                     | 0.50              |
| 31:YH:4:ILE:HG13   | 31:YH:6:ARG:NE     | 2.26                     | 0.50              |
| 41:YV:61:VAL:HA    | 41:YV:94:LEU:HD23  | 1.93                     | 0.50              |
| 1:QA:485:G:H1'     | 1:QA:486:U:H5      | 1.77                     | 0.50              |
| 1:QA:757:U:O2'     | 1:QA:879:C:O2      | 2.29                     | 0.50              |
| 4:QD:33:MET:CE     | 4:QD:37:PRO:HA     | 2.41                     | 0.50              |
| 13:QM:92:HIS:HD2   | 13:QM:110:ARG:HH21 | 1.58                     | 0.50              |
| 23:QW:19:G:P       | 23:QW:60:U:H3      | 2.33                     | 0.50              |
| 25:RA:1153:C:H2'   | 25:RA:1154:G:O4'   | 2.12                     | 0.50              |
| 33:RN:34:LEU:O     | 33:RN:49:GLY:HA3   | 2.12                     | 0.50              |
| 36:RQ:20:ALA:HB1   | 36:RQ:99:PRO:HD2   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:RS:67:ARG:O    | 38:RS:71:ARG:HG3   | 2.12                     | 0.50              |
| 39:RT:42:ILE:H    | 39:RT:42:ILE:HD12  | 1.77                     | 0.50              |
| 4:QD:194:LEU:HD12 | 6:XF:17:SER:OG     | 2.12                     | 0.50              |
| 13:XM:49:THR:HB   | 13:XM:52:GLU:H     | 1.77                     | 0.50              |
| 20:XT:64:ASP:HA   | 20:XT:67:ALA:HB3   | 1.93                     | 0.50              |
| 25:YA:1069:A:H4'  | 25:YA:1070:A:H5''  | 1.93                     | 0.50              |
| 25:YA:2071:A:H2'  | 25:YA:2072:G:H8    | 1.76                     | 0.50              |
| 25:YA:1803:A:H4'  | 27:YD:259:THR:HG23 | 1.93                     | 0.50              |
| 29:YF:108:LYS:O   | 29:YF:112:MET:HG3  | 2.12                     | 0.50              |
| 33:YN:58:ASP:N    | 33:YN:58:ASP:OD1   | 2.45                     | 0.50              |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:N     | 2.27                     | 0.50              |
| 43:YX:60:ARG:HH22 | 53:Y7:47:ARG:HH12  | 1.60                     | 0.50              |
| 1:QA:164:U:H2'    | 1:QA:165:C:C6      | 2.47                     | 0.49              |
| 1:QA:56:U:H2'     | 1:QA:57:G:H8       | 1.76                     | 0.49              |
| 3:QC:79:ARG:HD2   | 11:XK:99:GLN:HE22  | 1.71                     | 0.49              |
| 6:QF:17:SER:C     | 6:QF:19:LEU:N      | 2.64                     | 0.49              |
| 12:QL:24:VAL:HG13 | 12:QL:98:TYR:HE1   | 1.76                     | 0.49              |
| 37:RR:33:ARG:HH12 | 51:R5:57:VAL:HG23  | 1.75                     | 0.49              |
| 25:RA:2030:A:H4'  | 25:RA:2031:A:C8    | 2.47                     | 0.49              |
| 25:RA:2287:A:N6   | 25:RA:2344:U:C2    | 2.80                     | 0.49              |
| 25:RA:2566:A:H4'  | 25:RA:2567:G:O5'   | 2.12                     | 0.49              |
| 25:RA:654(A):G:N2 | 25:RA:654(T):C:C2  | 2.79                     | 0.49              |
| 26:RB:5:C:O2'     | 26:RB:27:C:O2      | 2.30                     | 0.49              |
| 29:RF:9:ILE:HD11  | 29:RF:125:LEU:HG   | 1.94                     | 0.49              |
| 37:RR:44:LEU:HD22 | 37:RR:48:VAL:HG23  | 1.94                     | 0.49              |
| 39:RT:34:VAL:HG12 | 39:RT:36:GLU:HG2   | 1.94                     | 0.49              |
| 39:RT:41:ARG:CB   | 39:RT:41:ARG:NH1   | 2.73                     | 0.49              |
| 1:XA:1016:A:H2'   | 1:XA:1017:G:O4'    | 2.12                     | 0.49              |
| 15:XO:67:LEU:HB3  | 15:XO:78:TYR:HE1   | 1.77                     | 0.49              |
| 23:XW:57:G:H2'    | 23:XW:58:A:H5'     | 1.94                     | 0.49              |
| 54:Y8:25:MET:O    | 54:Y8:47:LYS:NZ    | 2.44                     | 0.49              |
| 25:YA:1689:A:H62  | 25:YA:1698:A:H2    | 1.58                     | 0.49              |
| 25:YA:2340:G:H2'  | 25:YA:2341:G:C8    | 2.47                     | 0.49              |
| 25:YA:2884:U:C2   | 51:Y5:51:TYR:HE1   | 2.30                     | 0.49              |
| 28:YE:103:ASP:OD1 | 28:YE:201:THR:HG23 | 2.12                     | 0.49              |
| 25:YA:1012:U:O4   | 33:YN:25:ARG:HA    | 2.12                     | 0.49              |
| 40:YU:83:LEU:HG   | 40:YU:88:ILE:HG13  | 1.93                     | 0.49              |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:HB    | 1.76                     | 0.49              |
| 1:QA:1065:U:O2'   | 1:QA:1066:C:OP2    | 2.24                     | 0.49              |
| 1:QA:1218:C:H2'   | 1:QA:1219:U:C6     | 2.47                     | 0.49              |
| 1:QA:589:C:N4     | 1:QA:650:G:H1      | 2.06                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:162:ILE:HD11  | 2:QB:184:VAL:HG22  | 1.93                     | 0.49              |
| 2:QB:235:SER:OG    | 2:QB:236:TYR:N     | 2.46                     | 0.49              |
| 3:QC:157:ILE:HD11  | 3:QC:166:GLU:HB2   | 1.94                     | 0.49              |
| 8:QH:9:MET:HG3     | 8:QH:26:VAL:HG21   | 1.94                     | 0.49              |
| 9:QI:46:ALA:HB2    | 9:QI:74:ILE:HG23   | 1.94                     | 0.49              |
| 25:RA:2601:C:H2'   | 25:RA:2603:G:C8    | 2.47                     | 0.49              |
| 31:RH:155:SER:OG   | 31:RH:156:ALA:N    | 2.45                     | 0.49              |
| 36:RQ:69:PHE:CD1   | 36:RQ:70:PRO:HD2   | 2.46                     | 0.49              |
| 36:RQ:11:LYS:HE2   | 36:RQ:86:GLY:O     | 2.11                     | 0.49              |
| 38:RS:15:ARG:NH1   | 38:RS:25:ARG:HH21  | 2.11                     | 0.49              |
| 43:RX:26:TYR:HB3   | 43:RX:92:LEU:HD12  | 1.93                     | 0.49              |
| 1:XA:1301:U:H3'    | 1:XA:1302:U:H5'    | 1.94                     | 0.49              |
| 11:XK:82:VAL:HB    | 11:XK:108:ILE:HG12 | 1.94                     | 0.49              |
| 19:XS:41:VAL:HB    | 19:XS:42:PRO:CA    | 2.42                     | 0.49              |
| 46:Y0:70:GLN:OE1   | 46:Y0:72:ARG:HD3   | 2.12                     | 0.49              |
| 53:Y7:5:TRP:NE1    | 53:Y7:7:PRO:HG3    | 2.27                     | 0.49              |
| 25:YA:278:A:H2'    | 25:YA:279:C:C6     | 2.47                     | 0.49              |
| 28:YE:35:GLN:HG2   | 28:YE:37:ARG:HE    | 1.77                     | 0.49              |
| 33:YN:7:LYS:HD2    | 33:YN:7:LYS:N      | 2.27                     | 0.49              |
| 35:YP:126:VAL:HG13 | 35:YP:145:PRO:HB2  | 1.94                     | 0.49              |
| 1:QA:1201:A:O2'    | 1:QA:1202:G:O5'    | 2.29                     | 0.49              |
| 1:QA:946:A:H61     | 1:QA:1234:C:H42    | 1.60                     | 0.49              |
| 2:QB:96:ARG:H      | 2:QB:96:ARG:HD2    | 1.76                     | 0.49              |
| 3:QC:14:ILE:HG12   | 3:QC:15:THR:N      | 2.27                     | 0.49              |
| 1:QA:1226:C:O2'    | 13:QM:103:THR:O    | 2.25                     | 0.49              |
| 14:QN:15:LYS:HD2   | 14:QN:16:PHE:CE2   | 2.47                     | 0.49              |
| 14:QN:24:CYS:HB3   | 14:QN:29:ARG:H     | 1.78                     | 0.49              |
| 20:QT:79:ARG:O     | 20:QT:83:ARG:HG3   | 2.12                     | 0.49              |
| 25:RA:1441:G:H2'   | 25:RA:1442:G:H8    | 1.77                     | 0.49              |
| 25:RA:796:C:H2'    | 25:RA:797:C:C6     | 2.47                     | 0.49              |
| 26:RB:78:A:H2'     | 26:RB:79:C:O4'     | 2.12                     | 0.49              |
| 27:RD:175:LEU:HD12 | 27:RD:185:VAL:HG21 | 1.93                     | 0.49              |
| 32:RI:5:LEU:HD23   | 32:RI:9:LEU:HD11   | 1.94                     | 0.49              |
| 43:RX:27:THR:HB    | 43:RX:80:ILE:HB    | 1.93                     | 0.49              |
| 9:XI:40:LEU:C      | 9:XI:42:ARG:H      | 2.15                     | 0.49              |
| 12:XL:71:PRO:O     | 12:XL:102:ARG:HD3  | 2.12                     | 0.49              |
| 12:XL:62:SER:HB2   | 12:XL:64:TYR:HD1   | 1.76                     | 0.49              |
| 14:XN:23:ARG:NH1   | 14:XN:30:ALA:HB2   | 2.27                     | 0.49              |
| 25:YA:102:G:H4'    | 25:YA:103:A:O5'    | 2.11                     | 0.49              |
| 25:YA:2795:G:H3'   | 25:YA:2797:U:C5'   | 2.42                     | 0.49              |
| 28:YE:73:GLU:HG3   | 28:YE:74:PRO:HD2   | 1.92                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1288:A:N1     | 1:QA:1371:G:H1'    | 2.27                     | 0.49              |
| 3:QC:14:ILE:HG12   | 3:QC:15:THR:H      | 1.76                     | 0.49              |
| 3:QC:73:PRO:O      | 3:QC:76:VAL:HG22   | 2.12                     | 0.49              |
| 4:QD:29:PRO:O      | 4:QD:30:LYS:HB3    | 2.11                     | 0.49              |
| 18:QR:26:LEU:HD22  | 18:QR:42:ARG:HD2   | 1.94                     | 0.49              |
| 19:QS:68:GLY:N     | 50:R4:59:PHE:HE1   | 2.08                     | 0.49              |
| 22:QV:3:G:HO2'     | 22:QV:4:G:H8       | 1.58                     | 0.49              |
| 25:RA:1791:A:H5'   | 27:RD:206:LEU:HD12 | 1.95                     | 0.49              |
| 25:RA:229:A:H4'    | 25:RA:229:A:OP1    | 2.12                     | 0.49              |
| 25:RA:2377:A:H2'   | 25:RA:2378:A:C8    | 2.48                     | 0.49              |
| 30:RG:115:ARG:NH2  | 30:RG:137:GLU:OE1  | 2.46                     | 0.49              |
| 30:RG:60:LEU:O     | 30:RG:64:THR:HG22  | 2.11                     | 0.49              |
| 32:RI:2:LYS:HA     | 32:RI:20:ASP:HA    | 1.95                     | 0.49              |
| 43:RX:40:LYS:O     | 43:RX:42:ALA:N     | 2.45                     | 0.49              |
| 45:RZ:102:LEU:HB3  | 45:RZ:104:PHE:HE1  | 1.78                     | 0.49              |
| 50:Y4:15:ILE:HD13  | 50:Y4:15:ILE:H     | 1.76                     | 0.49              |
| 25:YA:1081:U:H3'   | 25:YA:1082:U:H4'   | 1.94                     | 0.49              |
| 25:YA:340:A:H2'    | 25:YA:341:G:O4'    | 2.12                     | 0.49              |
| 26:YB:41:U:C4      | 30:YG:70:VAL:HG23  | 2.48                     | 0.49              |
| 40:YU:61:TRP:CD2   | 40:YU:94:ASN:HA    | 2.47                     | 0.49              |
| 1:QA:1336:C:O2'    | 1:QA:1337:G:O5'    | 2.30                     | 0.49              |
| 4:QD:129:ASN:HA    | 4:QD:145:GLU:HB2   | 1.94                     | 0.49              |
| 7:QG:20:ASP:HB3    | 7:QG:23:VAL:HG23   | 1.94                     | 0.49              |
| 51:R5:40:LYS:HE2   | 51:R5:47:PRO:HD2   | 1.92                     | 0.49              |
| 53:R7:31:LEU:HD22  | 53:R7:42:LEU:HD13  | 1.95                     | 0.49              |
| 25:RA:1805:U:O2    | 27:RD:50:THR:HB    | 2.12                     | 0.49              |
| 25:RA:404:C:H1'    | 25:RA:405:U:OP2    | 2.13                     | 0.49              |
| 25:RA:813:U:H2'    | 25:RA:814:C:C6     | 2.48                     | 0.49              |
| 27:RD:35:LYS:HZ1   | 27:RD:65:ILE:HA    | 1.76                     | 0.49              |
| 29:RF:132:VAL:HG23 | 29:RF:133:ASN:OD1  | 2.12                     | 0.49              |
| 13:QM:3:ARG:CZ     | 30:RG:113:ARG:HH21 | 2.26                     | 0.49              |
| 33:RN:134:ARG:N    | 33:RN:135:PRO:HD3  | 2.28                     | 0.49              |
| 25:RA:2415:G:H4'   | 35:RP:67:MET:N     | 2.28                     | 0.49              |
| 13:XM:20:THR:C     | 13:XM:22:ILE:H     | 2.16                     | 0.49              |
| 16:XP:28:ARG:NH1   | 16:XP:29:ASP:OD2   | 2.45                     | 0.49              |
| 52:Y6:41:PRO:HD2   | 52:Y6:46:HIS:N     | 2.28                     | 0.49              |
| 25:YA:1348:G:H2'   | 25:YA:1349:A:H5''  | 1.94                     | 0.49              |
| 25:YA:888:C:H3'    | 25:YA:889:C:C4'    | 2.40                     | 0.49              |
| 27:YD:76:PRO:HG2   | 27:YD:98:VAL:HG21  | 1.93                     | 0.49              |
| 33:YN:17:ASP:O     | 33:YN:56:ASN:HB2   | 2.12                     | 0.49              |
| 33:YN:34:LEU:HD21  | 33:YN:120:LEU:HB2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:YX:53:LYS:HB3  | 43:YX:82:GLN:HB3   | 1.93                     | 0.49              |
| 1:QA:1104:G:H4'   | 2:QB:111:ARG:NH1   | 2.28                     | 0.49              |
| 2:QB:204:ASN:ND2  | 2:QB:206:ASP:O     | 2.45                     | 0.49              |
| 1:QA:255:G:H1'    | 17:QQ:16:GLN:NE2   | 2.28                     | 0.49              |
| 17:QQ:18:THR:HG23 | 17:QQ:69:LYS:HE3   | 1.94                     | 0.49              |
| 6:QF:97:PHE:O     | 18:QR:31:LEU:HD23  | 2.12                     | 0.49              |
| 19:QS:41:VAL:HA   | 19:QS:44:MET:HG3   | 1.93                     | 0.49              |
| 52:R6:15:GLU:CD   | 52:R6:41:PRO:HB3   | 2.32                     | 0.49              |
| 25:RA:2008:C:H2'  | 25:RA:2009:G:H8    | 1.78                     | 0.49              |
| 25:RA:2505:G:OP1  | 56:Z7:1:T17:H47    | 2.13                     | 0.49              |
| 25:RA:321:G:OP1   | 29:RF:135:LYS:NZ   | 2.36                     | 0.49              |
| 30:RG:110:ALA:HB1 | 30:RG:140:ILE:HD12 | 1.94                     | 0.49              |
| 39:RT:16:ARG:HD3  | 39:RT:19:LEU:HD11  | 1.93                     | 0.49              |
| 40:RU:92:ARG:O    | 40:RU:92:ARG:HG2   | 2.13                     | 0.49              |
| 13:XM:14:ARG:HG2  | 13:XM:17:VAL:HG23  | 1.94                     | 0.49              |
| 25:YA:1858:G:O2'  | 25:YA:1884:A:N6    | 2.44                     | 0.49              |
| 25:YA:807:U:H2'   | 25:YA:808:G:C8     | 2.47                     | 0.49              |
| 27:YD:27:THR:HG21 | 27:YD:83:GLU:HG2   | 1.94                     | 0.49              |
| 25:YA:691:C:O4'   | 27:YD:43:ARG:NH2   | 2.46                     | 0.49              |
| 30:YG:67:LYS:HZ1  | 50:Y4:1:MET:HB2    | 1.78                     | 0.49              |
| 40:YU:95:LEU:HD22 | 41:YV:4:ILE:HD12   | 1.93                     | 0.49              |
| 43:YX:57:LEU:HD11 | 43:YX:78:LYS:HD2   | 1.94                     | 0.49              |
| 1:QA:1152:A:H5''  | 10:QJ:13:HIS:CD2   | 2.48                     | 0.49              |
| 1:QA:1213:A:C6    | 1:QA:1215:G:H1'    | 2.48                     | 0.49              |
| 1:QA:570:G:O6     | 1:QA:865:A:N6      | 2.44                     | 0.49              |
| 3:QC:47:LEU:HD23  | 3:QC:68:VAL:HG11   | 1.94                     | 0.49              |
| 8:QH:95:VAL:HB    | 8:QH:99:GLU:O      | 2.13                     | 0.49              |
| 49:R3:6:VAL:HG13  | 49:R3:56:VAL:HG13  | 1.93                     | 0.49              |
| 52:R6:14:THR:O    | 52:R6:49:HIS:HA    | 2.12                     | 0.49              |
| 25:RA:1994:C:P    | 28:RE:127:ASP:HB2  | 2.52                     | 0.49              |
| 25:RA:2527:C:H5'' | 55:R9:30:PRO:HB2   | 1.94                     | 0.49              |
| 25:RA:2790:A:H2'  | 25:RA:2791:C:H5''  | 1.95                     | 0.49              |
| 25:RA:2795:G:H3'  | 25:RA:2797:U:C5'   | 2.43                     | 0.49              |
| 27:RD:228:PRO:HD3 | 27:RD:234:GLY:C    | 2.33                     | 0.49              |
| 44:RY:47:LYS:HG2  | 44:RY:60:PHE:HD1   | 1.76                     | 0.49              |
| 2:XB:24:TRP:CZ3   | 2:XB:26:PRO:HA     | 2.48                     | 0.49              |
| 25:YA:2232:U:P    | 47:Y1:40:ARG:HH12  | 2.35                     | 0.49              |
| 25:YA:2071:A:H2'  | 25:YA:2072:G:C8    | 2.48                     | 0.49              |
| 25:YA:583:G:OP2   | 40:YU:10:ARG:HD2   | 2.13                     | 0.49              |
| 28:YE:179:GLU:HB3 | 28:YE:181:LEU:HD23 | 1.94                     | 0.49              |
| 30:YG:94:LEU:HD12 | 30:YG:99:MET:HA    | 1.95                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1015:A:H2'   | 1:QA:1016:A:C8     | 2.48                     | 0.49              |
| 1:QA:191:G:O2'    | 20:QT:101:GLY:O    | 2.30                     | 0.49              |
| 2:QB:178:ARG:NH2  | 8:QH:74:PRO:HG3    | 2.28                     | 0.49              |
| 13:QM:23:TYR:HE1  | 13:QM:70:LEU:HD12  | 1.77                     | 0.49              |
| 52:R6:25:LYS:HE2  | 52:R6:27:LYS:HD3   | 1.94                     | 0.49              |
| 25:RA:1231:G:H2'  | 25:RA:1232:G:C8    | 2.47                     | 0.49              |
| 25:RA:1533:C:H42  | 25:RA:1538:G:H1    | 1.60                     | 0.49              |
| 25:RA:192:C:O2'   | 25:RA:802:A:N3     | 2.42                     | 0.49              |
| 25:RA:900:A:H3'   | 25:RA:901:A:H8     | 1.78                     | 0.49              |
| 26:RB:15:A:OP1    | 26:RB:107:U:O2'    | 2.28                     | 0.49              |
| 28:RE:70:ALA:O    | 28:RE:72:VAL:N     | 2.46                     | 0.49              |
| 29:RF:178:PRO:HG2 | 29:RF:179:GLU:OE2  | 2.13                     | 0.49              |
| 1:XA:690:G:H2'    | 1:XA:691:G:O4'     | 2.12                     | 0.49              |
| 3:XC:148:GLY:HA3  | 3:XC:172:ARG:O     | 2.12                     | 0.49              |
| 1:XA:923:A:OP1    | 5:XE:21:ALA:HB2    | 2.13                     | 0.49              |
| 4:QD:195:ALA:O    | 6:XF:16:GLN:CB     | 2.61                     | 0.49              |
| 10:XJ:49:VAL:HG22 | 14:XN:41:ARG:HB2   | 1.94                     | 0.49              |
| 13:XM:81:LEU:HD13 | 13:XM:88:ARG:HD2   | 1.94                     | 0.49              |
| 1:XA:267:C:OP1    | 17:XQ:67:LYS:HB2   | 2.13                     | 0.49              |
| 20:XT:89:ARG:NH2  | 20:XT:104:LEU:HD11 | 2.27                     | 0.49              |
| 25:YA:943:U:OP2   | 35:YP:36:LYS:NZ    | 2.42                     | 0.49              |
| 31:YH:98:LEU:HD13 | 31:YH:125:VAL:HB   | 1.94                     | 0.49              |
| 1:QA:1004:A:H1'   | 1:QA:1036:G:N2     | 2.27                     | 0.49              |
| 1:QA:1356:G:H2'   | 1:QA:1357:A:C8     | 2.47                     | 0.49              |
| 1:QA:148:G:H1     | 1:QA:174:C:H42     | 1.61                     | 0.49              |
| 2:QB:21:ARG:O     | 2:QB:23:ARG:N      | 2.46                     | 0.49              |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:H     | 1.78                     | 0.49              |
| 46:R0:32:ARG:H    | 46:R0:35:ASN:ND2   | 2.11                     | 0.49              |
| 25:RA:1209:G:O2'  | 25:RA:1237:A:N1    | 2.33                     | 0.49              |
| 25:RA:2364:C:OP1  | 46:R0:55:ARG:NH1   | 2.46                     | 0.49              |
| 29:RF:24:LEU:HD23 | 29:RF:115:ALA:HA   | 1.95                     | 0.49              |
| 31:RH:4:ILE:HG13  | 31:RH:6:ARG:NE     | 2.28                     | 0.49              |
| 36:RQ:89:ASN:O    | 36:RQ:91:GLU:N     | 2.45                     | 0.49              |
| 1:XA:200:G:H1     | 1:XA:217:C:H42     | 1.60                     | 0.49              |
| 1:XA:737:A:H2'    | 1:XA:738:C:C6      | 2.47                     | 0.49              |
| 52:Y6:21:TYR:HE2  | 52:Y6:53:LYS:HE3   | 1.77                     | 0.49              |
| 25:YA:1754:C:P    | 39:YT:96:ARG:NH1   | 2.86                     | 0.49              |
| 25:YA:573:G:O2'   | 25:YA:574:C:H3'    | 2.13                     | 0.49              |
| 27:YD:170:GLY:C   | 27:YD:172:TYR:H    | 2.16                     | 0.49              |
| 4:QD:166:LYS:HD3  | 27:YD:188:GLU:OE2  | 2.12                     | 0.49              |
| 28:YE:24:THR:HG22 | 28:YE:24:THR:O     | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:YY:86:ARG:HB2  | 44:YY:95:LYS:HD2  | 1.94                     | 0.49              |
| 1:QA:1466:C:H2'   | 1:QA:1467:G:O4'   | 2.12                     | 0.49              |
| 1:QA:769:G:H4'    | 1:QA:1513:A:H4'   | 1.95                     | 0.49              |
| 1:QA:64:G:H4'     | 1:QA:65:U:H5'     | 1.95                     | 0.49              |
| 1:QA:950:U:H2'    | 1:QA:951:G:C8     | 2.48                     | 0.49              |
| 10:QJ:24:VAL:HG21 | 10:QJ:37:PRO:HD3  | 1.95                     | 0.49              |
| 12:QL:58:VAL:O    | 12:QL:65:GLU:HA   | 2.13                     | 0.49              |
| 19:QS:77:THR:HG22 | 19:QS:78:ARG:HD3  | 1.95                     | 0.49              |
| 25:RA:2466:C:OP1  | 55:R9:4:ARG:HB2   | 2.13                     | 0.49              |
| 30:RG:54:GLU:HA   | 30:RG:57:ALA:HB3  | 1.94                     | 0.49              |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:CD  | 2.43                     | 0.49              |
| 2:XB:47:THR:HA    | 2:XB:202:PRO:HG2  | 1.95                     | 0.49              |
| 5:XE:31:LEU:HD23  | 5:XE:45:PHE:HD1   | 1.78                     | 0.49              |
| 6:XF:10:LEU:HD22  | 6:XF:61:LEU:HD11  | 1.94                     | 0.49              |
| 6:XF:19:LEU:HD21  | 6:XF:59:TYR:CE1   | 2.47                     | 0.49              |
| 6:XF:97:PHE:HD1   | 18:XR:31:LEU:HD21 | 1.78                     | 0.49              |
| 10:XJ:35:SER:OG   | 10:XJ:73:ASP:HB2  | 2.13                     | 0.49              |
| 46:Y0:53:MET:HA   | 46:Y0:58:THR:O    | 2.13                     | 0.49              |
| 25:YA:2344:U:OP1  | 52:Y6:38:LYS:HD3  | 2.13                     | 0.49              |
| 52:Y6:41:PRO:O    | 52:Y6:45:LYS:HE3  | 2.12                     | 0.49              |
| 25:YA:1384:A:N3   | 25:YA:1405:U:H1'  | 2.27                     | 0.49              |
| 25:YA:1427:A:H4'  | 25:YA:1428:C:O5'  | 2.12                     | 0.49              |
| 25:YA:1311:G:N2   | 25:YA:1603:A:H62  | 2.11                     | 0.49              |
| 29:YF:185:ASP:OD1 | 29:YF:188:ARG:NH1 | 2.35                     | 0.49              |
| 32:YI:76:THR:OG1  | 32:YI:139:GLN:OE1 | 2.31                     | 0.49              |
| 34:YO:4:PRO:O     | 34:YO:5:GLN:HB2   | 2.11                     | 0.49              |
| 40:YU:98:LEU:O    | 40:YU:102:GLU:N   | 2.37                     | 0.49              |
| 1:QA:1159:U:C6    | 1:QA:1182:G:H1'   | 2.47                     | 0.48              |
| 1:QA:474:G:H5'    | 16:QP:81:ARG:HG3  | 1.94                     | 0.48              |
| 21:QU:5:ASP:O     | 21:QU:11:GLY:HA3  | 2.13                     | 0.48              |
| 23:QW:7:A:N6      | 23:QW:66:U:H3     | 2.10                     | 0.48              |
| 25:RA:1204:A:H1'  | 25:RA:1206:G:C8   | 2.48                     | 0.48              |
| 25:RA:2037:G:H2'  | 25:RA:2038:G:C8   | 2.48                     | 0.48              |
| 44:RY:47:LYS:HG2  | 44:RY:60:PHE:CD1  | 2.48                     | 0.48              |
| 1:XA:1129:C:H4'   | 1:XA:1130:A:H8    | 1.77                     | 0.48              |
| 1:XA:1495:U:H2'   | 1:XA:1496:C:C6    | 2.48                     | 0.48              |
| 1:XA:539:A:OP1    | 12:XL:114:LYS:NZ  | 2.37                     | 0.48              |
| 1:XA:779:C:H2'    | 1:XA:780:A:O4'    | 2.13                     | 0.48              |
| 1:XA:950:U:H2'    | 1:XA:951:G:H8     | 1.78                     | 0.48              |
| 1:XA:973:G:H3'    | 1:XA:974:A:C5'    | 2.42                     | 0.48              |
| 3:XC:79:ARG:HH12  | 3:XC:82:GLU:HG3   | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:XE:33:VAL:HG11   | 5:XE:109:ILE:HA    | 1.95                     | 0.48              |
| 5:XE:10:MET:SD     | 5:XE:13:ILE:HD13   | 2.53                     | 0.48              |
| 25:YA:1045:A:O2'   | 25:YA:1046:A:OP2   | 2.28                     | 0.48              |
| 25:YA:2776:A:H4'   | 25:YA:2777:G:O5'   | 2.12                     | 0.48              |
| 25:YA:654(A):G:H8  | 25:YA:654(A):G:OP2 | 1.96                     | 0.48              |
| 27:YD:248:SER:OG   | 27:YD:252:TRP:CD1  | 2.57                     | 0.48              |
| 27:YD:61:LEU:O     | 27:YD:63:ARG:NH1   | 2.45                     | 0.48              |
| 29:YF:176:LEU:HD21 | 29:YF:181:LEU:HA   | 1.94                     | 0.48              |
| 31:YH:55:PRO:HG2   | 31:YH:61:HIS:CE1   | 2.48                     | 0.48              |
| 36:YQ:104:PHE:CE2  | 36:YQ:125:LEU:HD11 | 2.41                     | 0.48              |
| 1:QA:510:A:OP2     | 4:QD:49:ARG:NH2    | 2.45                     | 0.48              |
| 1:QA:35:G:O2'      | 12:QL:118:SER:O    | 2.31                     | 0.48              |
| 15:QO:16:ALA:HB1   | 15:QO:21:ASP:HB3   | 1.94                     | 0.48              |
| 25:RA:103:A:H8     | 25:RA:103:A:O5'    | 1.96                     | 0.48              |
| 25:RA:1412:A:H2'   | 25:RA:1413:G:O4'   | 2.13                     | 0.48              |
| 25:RA:1803:A:O2'   | 27:RD:259:THR:HG21 | 2.14                     | 0.48              |
| 25:RA:2119:A:N6    | 25:RA:2170:A:N7    | 2.61                     | 0.48              |
| 25:RA:783:A:H2'    | 25:RA:784:A:H4'    | 1.94                     | 0.48              |
| 29:RF:155:LEU:HD12 | 29:RF:174:VAL:HG22 | 1.94                     | 0.48              |
| 3:XC:134:ILE:HG23  | 3:XC:151:VAL:HB    | 1.94                     | 0.48              |
| 11:XK:59:TYR:CZ    | 11:XK:63:LEU:HD11  | 2.48                     | 0.48              |
| 16:XP:26:ARG:HH21  | 16:XP:31:LYS:HB3   | 1.77                     | 0.48              |
| 47:Y1:41:ARG:HG3   | 47:Y1:41:ARG:HH11  | 1.78                     | 0.48              |
| 25:YA:2227:A:H5''  | 27:YD:263:ARG:NH1  | 2.29                     | 0.48              |
| 25:YA:2693:A:H2'   | 25:YA:2694:G:H8    | 1.78                     | 0.48              |
| 25:YA:671:C:H2'    | 25:YA:672:C:H6     | 1.78                     | 0.48              |
| 27:YD:35:LYS:HD3   | 27:YD:63:ARG:CB    | 2.43                     | 0.48              |
| 30:YG:166:ASP:HA   | 30:YG:169:ALA:HB3  | 1.95                     | 0.48              |
| 25:YA:954:G:H5''   | 36:YQ:13:GLN:HB3   | 1.94                     | 0.48              |
| 39:YT:107:ASP:H    | 39:YT:110:ILE:HG22 | 1.78                     | 0.48              |
| 34:YO:76:ALA:HB3   | 39:YT:75:ILE:HD12  | 1.95                     | 0.48              |
| 42:YW:51:LEU:HD23  | 42:YW:105:VAL:HG11 | 1.94                     | 0.48              |
| 1:QA:1392:G:N2     | 1:QA:1502:A:H8     | 2.05                     | 0.48              |
| 2:QB:80:ILE:HG21   | 2:QB:212:GLN:HA    | 1.95                     | 0.48              |
| 7:QG:155:ARG:O     | 7:QG:155:ARG:NH2   | 2.46                     | 0.48              |
| 7:QG:57:GLU:OE1    | 7:QG:57:GLU:N      | 2.41                     | 0.48              |
| 12:QL:38:THR:O     | 12:QL:79:GLU:HG3   | 2.14                     | 0.48              |
| 25:RA:1777:U:H3    | 25:RA:1787:A:H61   | 1.61                     | 0.48              |
| 25:RA:686:G:N2     | 25:RA:788:A:H61    | 2.11                     | 0.48              |
| 28:RE:181:LEU:HD21 | 39:RT:7:ILE:HG23   | 1.95                     | 0.48              |
| 31:RH:41:MET:HG3   | 31:RH:54:ARG:HA    | 1.96                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1190:G:H5'   | 35:RP:32:THR:HA   | 1.95                     | 0.48              |
| 37:RR:2:ARG:HA     | 37:RR:5:LYS:HE3   | 1.95                     | 0.48              |
| 43:RX:39:ILE:O     | 43:RX:43:VAL:HG12 | 2.13                     | 0.48              |
| 2:XB:73:THR:OG1    | 2:XB:170:GLU:OE2  | 2.23                     | 0.48              |
| 1:XA:1359:C:OP2    | 14:XN:35:ARG:NH1  | 2.46                     | 0.48              |
| 25:YA:1026:U:H1'   | 25:YA:1027:A:O5'  | 2.12                     | 0.48              |
| 25:YA:1085:A:O2'   | 25:YA:1086:A:OP1  | 2.27                     | 0.48              |
| 25:YA:1408:C:H2'   | 25:YA:1409:C:C6   | 2.48                     | 0.48              |
| 25:YA:2335:A:HO2'  | 25:YA:2336:A:P    | 2.35                     | 0.48              |
| 25:YA:220:G:O2'    | 25:YA:233:A:N3    | 2.42                     | 0.48              |
| 31:YH:137:ASP:HB3  | 31:YH:140:LYS:HB3 | 1.94                     | 0.48              |
| 25:YA:2641:G:P     | 33:YN:83:LYS:HE3  | 2.53                     | 0.48              |
| 35:YP:135:LEU:HD13 | 35:YP:139:LYS:HE2 | 1.94                     | 0.48              |
| 35:YP:82:GLY:HA2   | 35:YP:113:LYS:O   | 2.12                     | 0.48              |
| 28:YE:111:ARG:HG2  | 37:YR:1:MET:SD    | 2.53                     | 0.48              |
| 1:QA:715:A:H2'     | 1:QA:716:A:C8     | 2.49                     | 0.48              |
| 1:QA:753:A:H4'     | 1:QA:754:C:O5'    | 2.12                     | 0.48              |
| 10:QJ:32:ALA:HB3   | 10:QJ:76:ASN:HB2  | 1.95                     | 0.48              |
| 13:QM:49:THR:HG22  | 13:QM:51:ALA:H    | 1.79                     | 0.48              |
| 47:R1:53:VAL:HB    | 47:R1:58:ILE:HD12 | 1.94                     | 0.48              |
| 25:RA:263:C:H2'    | 25:RA:264:C:O4'   | 2.13                     | 0.48              |
| 25:RA:626:U:H5''   | 25:RA:627:A:H5'   | 1.94                     | 0.48              |
| 25:RA:78:A:H2'     | 25:RA:79:G:C8     | 2.48                     | 0.48              |
| 31:RH:152:ARG:HH21 | 31:RH:153:LYS:HZ1 | 1.61                     | 0.48              |
| 37:RR:97:VAL:HG22  | 37:RR:114:VAL:CG2 | 2.43                     | 0.48              |
| 3:XC:7:PRO:O       | 3:XC:11:ARG:HG2   | 2.13                     | 0.48              |
| 11:XK:18:ARG:NH2   | 11:XK:35:PRO:O    | 2.45                     | 0.48              |
| 20:XT:93:GLU:OE1   | 20:XT:94:ALA:N    | 2.46                     | 0.48              |
| 25:YA:469:G:O6     | 53:Y7:37:LYS:NZ   | 2.38                     | 0.48              |
| 35:YP:46:LYS:HB3   | 35:YP:46:LYS:HE3  | 1.54                     | 0.48              |
| 41:YV:15:GLU:O     | 41:YV:18:LEU:HB2  | 2.14                     | 0.48              |
| 1:QA:1465:C:H2'    | 1:QA:1466:C:O4'   | 2.14                     | 0.48              |
| 3:QC:150:LYS:HG3   | 3:QC:169:ALA:HB2  | 1.96                     | 0.48              |
| 16:QP:43:LYS:HA    | 16:QP:48:TRP:HB3  | 1.95                     | 0.48              |
| 25:RA:1062:G:H2'   | 25:RA:1063:G:C8   | 2.48                     | 0.48              |
| 25:RA:2563:U:H1'   | 25:RA:2566:A:N6   | 2.29                     | 0.48              |
| 25:RA:372:G:H1'    | 25:RA:373:U:H5    | 1.78                     | 0.48              |
| 35:RP:58:THR:O     | 35:RP:61:ARG:CZ   | 2.61                     | 0.48              |
| 33:RN:4:TYR:O      | 40:RU:64:ARG:NH1  | 2.46                     | 0.48              |
| 44:RY:81:LYS:NZ    | 44:RY:98:VAL:HG11 | 2.28                     | 0.48              |
| 1:XA:170:U:H2'     | 1:XA:171:A:H8     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:C8   | 2.48                     | 0.48              |
| 3:XC:130:VAL:HG21 | 3:XC:157:ILE:HG23  | 1.94                     | 0.48              |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HG21  | 1.94                     | 0.48              |
| 5:XE:50:GLU:HG3   | 5:XE:52:PRO:HD2    | 1.95                     | 0.48              |
| 6:XF:35:ALA:HA    | 6:XF:67:MET:HB3    | 1.94                     | 0.48              |
| 9:XI:9:ARG:HB2    | 9:XI:14:VAL:HA     | 1.96                     | 0.48              |
| 25:YA:2756:U:OP2  | 55:Y9:19:ARG:NH2   | 2.46                     | 0.48              |
| 25:YA:2712:U:O2'  | 25:YA:2712(A):A:H8 | 1.96                     | 0.48              |
| 25:YA:278:A:O2'   | 25:YA:279:C:O4'    | 2.20                     | 0.48              |
| 26:YB:12:C:C2'    | 46:Y0:73:GLY:HA3   | 2.43                     | 0.48              |
| 35:YP:5:ASP:O     | 35:YP:6:LEU:O      | 2.31                     | 0.48              |
| 39:YT:102:ILE:HB  | 39:YT:110:ILE:HD13 | 1.95                     | 0.48              |
| 40:YU:60:LEU:O    | 40:YU:60:LEU:HD22  | 2.14                     | 0.48              |
| 43:YX:63:LYS:O    | 43:YX:64:LYS:HD2   | 2.14                     | 0.48              |
| 4:QD:100:ARG:NH2  | 4:QD:136:PRO:O     | 2.46                     | 0.48              |
| 9:QI:17:VAL:HG11  | 9:QI:81:ILE:HA     | 1.95                     | 0.48              |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:HA    | 1.95                     | 0.48              |
| 7:QG:149:ARG:CD   | 11:QK:59:TYR:CZ    | 2.97                     | 0.48              |
| 49:R3:4:LEU:O     | 49:R3:36:VAL:HA    | 2.13                     | 0.48              |
| 25:RA:1019:U:HO2' | 25:RA:1021:A:H2    | 1.60                     | 0.48              |
| 25:RA:858:U:O2    | 25:RA:2268:A:H2'   | 2.13                     | 0.48              |
| 25:RA:297:C:H2'   | 25:RA:298:G:O4'    | 2.13                     | 0.48              |
| 25:RA:643:A:N1    | 25:RA:2369:A:O2'   | 2.45                     | 0.48              |
| 35:RP:59:LEU:HA   | 35:RP:61:ARG:HE    | 1.76                     | 0.48              |
| 1:XA:537:G:H5''   | 12:XL:113:ARG:NH1  | 2.29                     | 0.48              |
| 2:XB:101:MET:HA   | 2:XB:108:ILE:HG13  | 1.95                     | 0.48              |
| 5:XE:6:PHE:CE1    | 5:XE:36:ASP:HB3    | 2.48                     | 0.48              |
| 6:XF:36:ARG:CZ    | 6:XF:38:GLU:HG2    | 2.44                     | 0.48              |
| 15:XO:70:LEU:HD11 | 15:XO:77:ARG:HG3   | 1.96                     | 0.48              |
| 51:Y5:41:PRO:O    | 51:Y5:44:THR:OG1   | 2.32                     | 0.48              |
| 25:YA:468:G:N7    | 53:Y7:39:ARG:NH2   | 2.59                     | 0.48              |
| 25:YA:1819:A:H4'  | 25:YA:1820:U:O5'   | 2.13                     | 0.48              |
| 25:YA:2081:C:H2'  | 25:YA:2082:A:H8    | 1.79                     | 0.48              |
| 25:YA:676:A:N1    | 25:YA:802:A:N1     | 2.61                     | 0.48              |
| 13:XM:11:ARG:NH2  | 30:YG:146:TYR:HD2  | 2.08                     | 0.48              |
| 35:YP:52:GLU:O    | 35:YP:55:ARG:HG2   | 2.14                     | 0.48              |
| 1:QA:238:G:OP1    | 17:QQ:25:ARG:NH2   | 2.46                     | 0.48              |
| 20:QT:12:ALA:O    | 20:QT:15:ARG:HB2   | 2.14                     | 0.48              |
| 11:QK:54:ARG:NH1  | 23:QW:39:U:O2'     | 2.41                     | 0.48              |
| 25:RA:223:A:N1    | 25:RA:407:G:O2'    | 2.42                     | 0.48              |
| 25:RA:2734:A:H5'  | 25:RA:2735:G:OP2   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:178:PRO:HB2  | 29:RF:201:VAL:HG11 | 1.94                     | 0.48              |
| 30:RG:81:LYS:O     | 30:RG:82:LEU:HB2   | 2.12                     | 0.48              |
| 35:RP:36:LYS:HB3   | 35:RP:40:SER:HB3   | 1.95                     | 0.48              |
| 38:RS:64:GLU:O     | 38:RS:68:GLN:HG3   | 2.14                     | 0.48              |
| 1:XA:411:A:N9      | 1:XA:413:G:H1'     | 2.28                     | 0.48              |
| 12:XL:47:LYS:HB3   | 12:XL:48:PRO:HD2   | 1.96                     | 0.48              |
| 52:Y6:27:LYS:HB2   | 52:Y6:27:LYS:NZ    | 2.28                     | 0.48              |
| 25:YA:1045:A:C5    | 25:YA:1111:A:N7    | 2.81                     | 0.48              |
| 25:YA:1220:A:OP2   | 40:YU:19:LYS:NZ    | 2.33                     | 0.48              |
| 35:YP:14:LYS:O     | 35:YP:16:ARG:HG2   | 2.13                     | 0.48              |
| 40:YU:97:ASP:OD2   | 40:YU:101:ARG:NH1  | 2.46                     | 0.48              |
| 40:YU:90:VAL:HG22  | 41:YV:39:LEU:HB3   | 1.96                     | 0.48              |
| 25:YA:874:G:H4'    | 45:YZ:118:GLN:OE1  | 2.13                     | 0.48              |
| 1:QA:745:C:OP1     | 1:QA:851:G:O2'     | 2.31                     | 0.48              |
| 1:QA:877:C:H5''    | 8:QH:88:LYS:HD3    | 1.95                     | 0.48              |
| 2:QB:163:PHE:HD1   | 2:QB:185:ILE:HG13  | 1.78                     | 0.48              |
| 4:QD:106:TYR:HE1   | 4:QD:112:VAL:O     | 1.97                     | 0.48              |
| 9:QI:40:LEU:O      | 9:QI:42:ARG:N      | 2.46                     | 0.48              |
| 1:QA:1310:G:OP2    | 13:QM:88:ARG:NH2   | 2.46                     | 0.48              |
| 25:RA:2186:G:H2'   | 25:RA:2187:G:H8    | 1.79                     | 0.48              |
| 25:RA:340:A:H2'    | 25:RA:341:G:O4'    | 2.13                     | 0.48              |
| 27:RD:25:THR:O     | 27:RD:27:THR:HG22  | 2.14                     | 0.48              |
| 29:RF:102:PRO:HB2  | 29:RF:105:VAL:HG23 | 1.95                     | 0.48              |
| 29:RF:197:ASP:N    | 29:RF:197:ASP:OD1  | 2.46                     | 0.48              |
| 30:RG:82:LEU:HD21  | 30:RG:88:ILE:HG13  | 1.96                     | 0.48              |
| 31:RH:86:GLU:N     | 31:RH:86:GLU:OE1   | 2.43                     | 0.48              |
| 37:RR:33:ARG:NH1   | 51:R5:57:VAL:HG21  | 2.29                     | 0.48              |
| 44:RY:51:VAL:O     | 44:RY:56:PRO:HA    | 2.14                     | 0.48              |
| 1:XA:662:G:H2'     | 1:XA:663:A:C8      | 2.48                     | 0.48              |
| 16:XP:22:THR:HA    | 16:XP:33:ILE:HG12  | 1.96                     | 0.48              |
| 25:YA:270(T):G:OP1 | 47:Y1:97:LEU:HD13  | 2.13                     | 0.48              |
| 25:YA:1101:U:H2'   | 25:YA:1102:C:C6    | 2.49                     | 0.48              |
| 25:YA:1287:A:N7    | 37:YR:107:ASP:HB2  | 2.28                     | 0.48              |
| 25:YA:1508:A:O2'   | 25:YA:1509:C:O4'   | 2.25                     | 0.48              |
| 25:YA:1537:C:H2'   | 25:YA:1538:G:C8    | 2.48                     | 0.48              |
| 25:YA:207:A:H2'    | 25:YA:208:C:O4'    | 2.14                     | 0.48              |
| 25:YA:2212:A:H1'   | 25:YA:2215:G:C5    | 2.48                     | 0.48              |
| 25:YA:28:A:H61     | 25:YA:512:G:H1'    | 1.78                     | 0.48              |
| 27:YD:254:THR:O    | 27:YD:254:THR:OG1  | 2.30                     | 0.48              |
| 27:YD:35:LYS:HZ1   | 27:YD:104:TYR:HB2  | 1.79                     | 0.48              |
| 38:YS:58:LEU:HD12  | 38:YS:68:GLN:OE1   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:YV:76:LYS:HB2   | 41:YV:81:TYR:HB3   | 1.95                     | 0.48              |
| 42:YW:67:ASP:OD1   | 42:YW:67:ASP:N     | 2.46                     | 0.48              |
| 44:YY:44:ILE:HG13  | 44:YY:45:VAL:N     | 2.28                     | 0.48              |
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8  | 2.49                     | 0.48              |
| 1:QA:1124:G:H3'    | 1:QA:1145:C:N4     | 2.29                     | 0.48              |
| 1:QA:703:G:H4'     | 1:QA:704:A:O5'     | 2.14                     | 0.48              |
| 7:QG:113:GLU:HG3   | 7:QG:119:ARG:HG2   | 1.94                     | 0.48              |
| 13:QM:57:ARG:HH11  | 13:QM:57:ARG:HB2   | 1.79                     | 0.48              |
| 22:QV:15:C:H5''    | 22:QV:16:C:H5      | 1.79                     | 0.48              |
| 50:R4:23:GLU:HG3   | 50:R4:25:TYR:CE2   | 2.49                     | 0.48              |
| 52:R6:18:ARG:HB2   | 52:R6:44:ARG:HH12  | 1.77                     | 0.48              |
| 54:R8:51:ALA:N     | 54:R8:53:PRO:HD2   | 2.29                     | 0.48              |
| 25:RA:2344:U:OP1   | 52:R6:38:LYS:HD3   | 2.13                     | 0.48              |
| 26:RB:13:A:N1      | 26:RB:69:G:O2'     | 2.36                     | 0.48              |
| 33:RN:7:LYS:HD2    | 33:RN:7:LYS:H      | 1.79                     | 0.48              |
| 1:XA:1157:A:H1'    | 1:XA:1158:C:C4     | 2.49                     | 0.48              |
| 1:XA:143:A:H2      | 1:XA:220:G:H1      | 1.62                     | 0.48              |
| 1:XA:1502:A:H2'    | 1:XA:1504:G:N7     | 2.29                     | 0.48              |
| 1:XA:164:U:H2'     | 1:XA:165:C:C6      | 2.49                     | 0.48              |
| 2:XB:204:ASN:ND2   | 2:XB:206:ASP:H     | 2.12                     | 0.48              |
| 1:XA:1060:C:C5     | 3:XC:2:GLY:HA2     | 2.49                     | 0.48              |
| 9:XI:114:TYR:N     | 9:XI:114:TYR:CD1   | 2.81                     | 0.48              |
| 1:XA:390:C:O3'     | 16:XP:28:ARG:NH2   | 2.46                     | 0.48              |
| 19:XS:39:THR:HG22  | 19:XS:40:ILE:H     | 1.78                     | 0.48              |
| 20:XT:98:PRO:O     | 20:XT:100:ILE:N    | 2.46                     | 0.48              |
| 38:YS:74:ALA:HB1   | 38:YS:107:GLU:HB3  | 1.96                     | 0.48              |
| 1:QA:134:A:H61     | 16:QP:25:ARG:NH1   | 2.12                     | 0.48              |
| 1:QA:692:U:N3      | 1:QA:695:A:OP2     | 2.39                     | 0.48              |
| 1:QA:757:U:H2'     | 1:QA:758:G:O4'     | 2.13                     | 0.48              |
| 12:QL:17:LYS:HG2   | 12:QL:19:ARG:HG2   | 1.94                     | 0.48              |
| 19:QS:26:GLY:O     | 19:QS:28:LYS:N     | 2.41                     | 0.48              |
| 23:QW:30:G:H2'     | 23:QW:31:A:H8      | 1.77                     | 0.48              |
| 25:RA:709:U:H3     | 25:RA:722:A:H61    | 1.60                     | 0.48              |
| 25:RA:898:C:H2'    | 25:RA:899:A:H5'    | 1.95                     | 0.48              |
| 29:RF:183:VAL:O    | 29:RF:187:VAL:HG23 | 2.13                     | 0.48              |
| 32:RI:13:GLY:HA3   | 32:RI:17:GLN:CD    | 2.33                     | 0.48              |
| 45:RZ:52:SER:O     | 45:RZ:54:HIS:N     | 2.46                     | 0.48              |
| 45:RZ:91:LEU:CD1   | 45:RZ:96:VAL:HG21  | 2.43                     | 0.48              |
| 12:XL:27:LEU:O     | 12:XL:29:GLY:N     | 2.46                     | 0.48              |
| 25:YA:2146:C:H4'   | 25:YA:2147:G:C8    | 2.49                     | 0.48              |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6  | 2.49                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:450:G:O6    | 25:YA:453:C:OP1    | 2.32                     | 0.48              |
| 25:YA:817:C:H2'   | 25:YA:818:G:O4'    | 2.14                     | 0.48              |
| 25:YA:2780:G:OP2  | 33:YN:118:LYS:HE2  | 2.14                     | 0.48              |
| 40:YU:92:ARG:CZ   | 41:YV:11:GLN:H     | 2.26                     | 0.48              |
| 44:YY:35:TYR:CD2  | 44:YY:69:ALA:HB3   | 2.49                     | 0.48              |
| 5:QE:69:VAL:O     | 5:QE:71:LEU:N      | 2.47                     | 0.47              |
| 10:QJ:78:ASN:O    | 10:QJ:82:ILE:HG12  | 2.14                     | 0.47              |
| 19:QS:68:GLY:O    | 50:R4:68:ARG:HD3   | 2.14                     | 0.47              |
| 35:RP:61:ARG:CD   | 54:R8:13:ARG:HD2   | 2.44                     | 0.47              |
| 25:RA:2050:C:N4   | 25:RA:2051:A:N1    | 2.62                     | 0.47              |
| 25:RA:2283:C:H2'  | 25:RA:2284:C:O4'   | 2.13                     | 0.47              |
| 25:RA:2331:G:O2'  | 46:R0:43:THR:HG22  | 2.14                     | 0.47              |
| 25:RA:724:U:H2'   | 25:RA:725:G:O4'    | 2.13                     | 0.47              |
| 25:RA:848:G:H2'   | 25:RA:849:A:C8     | 2.49                     | 0.47              |
| 26:RB:104:A:H2'   | 26:RB:105:G:O4'    | 2.14                     | 0.47              |
| 29:RF:167:ALA:HB1 | 29:RF:173:VAL:HG11 | 1.95                     | 0.47              |
| 31:RH:154:PRO:HD3 | 31:RH:162:ILE:H    | 1.77                     | 0.47              |
| 25:RA:870:A:OP1   | 36:RQ:6:ARG:NE     | 2.47                     | 0.47              |
| 39:RT:41:ARG:CB   | 39:RT:41:ARG:HH11  | 2.27                     | 0.47              |
| 43:RX:83:VAL:HG11 | 43:RX:87:GLN:HB2   | 1.96                     | 0.47              |
| 1:XA:509:A:H2'    | 1:XA:510:A:C8      | 2.49                     | 0.47              |
| 19:XS:4:SER:N     | 50:Y4:67:TYR:CE2   | 2.82                     | 0.47              |
| 25:YA:1053:C:H42  | 25:YA:1106:G:H1    | 1.60                     | 0.47              |
| 25:YA:1357:U:H2'  | 25:YA:1358:G:O4'   | 2.13                     | 0.47              |
| 25:YA:1910:G:H1   | 25:YA:1920:C:H42   | 1.62                     | 0.47              |
| 25:YA:2291:U:H2'  | 25:YA:2292:C:C6    | 2.48                     | 0.47              |
| 25:YA:2777:G:OP2  | 25:YA:2781:A:O2'   | 2.20                     | 0.47              |
| 25:YA:729:G:C6    | 27:YD:208:LYS:HB2  | 2.49                     | 0.47              |
| 27:YD:28:GLU:HB2  | 27:YD:29:PRO:CD    | 2.44                     | 0.47              |
| 29:YF:36:VAL:HG11 | 29:YF:183:VAL:HG11 | 1.95                     | 0.47              |
| 32:YI:69:LYS:HG3  | 32:YI:136:VAL:HB   | 1.96                     | 0.47              |
| 33:YN:134:ARG:N   | 33:YN:135:PRO:HD3  | 2.29                     | 0.47              |
| 35:YP:98:GLU:HA   | 35:YP:101:VAL:HB   | 1.96                     | 0.47              |
| 38:YS:65:VAL:O    | 38:YS:69:VAL:HG12  | 2.14                     | 0.47              |
| 41:YV:44:LYS:O    | 41:YV:46:VAL:HG12  | 2.13                     | 0.47              |
| 1:QA:1391:U:H2'   | 1:QA:1392:G:C8     | 2.48                     | 0.47              |
| 1:QA:143:A:H2     | 1:QA:220:G:H1      | 1.62                     | 0.47              |
| 2:QB:97:TRP:CH2   | 2:QB:173:ALA:HA    | 2.49                     | 0.47              |
| 2:QB:85:ALA:HB3   | 2:QB:92:TYR:HD2    | 1.79                     | 0.47              |
| 20:QT:75:ASN:OD1  | 20:QT:75:ASN:N     | 2.40                     | 0.47              |
| 23:QW:38:A:H2'    | 23:QW:39:U:H5'     | 1.96                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:R2:41:ILE:HD11  | 48:R2:44:LEU:HD12 | 1.96                     | 0.47              |
| 26:RB:43:C:H5'     | 50:R4:1:MET:HA    | 1.95                     | 0.47              |
| 30:RG:145:THR:O    | 30:RG:147:ASP:N   | 2.47                     | 0.47              |
| 32:RI:128:LEU:HD13 | 32:RI:128:LEU:HA  | 1.56                     | 0.47              |
| 32:RI:49:ALA:O     | 32:RI:52:ARG:HG2  | 2.14                     | 0.47              |
| 35:RP:127:ALA:HB3  | 35:RP:130:PHE:CZ  | 2.49                     | 0.47              |
| 25:RA:297:C:H5''   | 44:RY:85:VAL:HG21 | 1.95                     | 0.47              |
| 3:XC:70:VAL:HG12   | 3:XC:72:LYS:H     | 1.79                     | 0.47              |
| 1:XA:405:U:O4      | 4:XD:2:GLY:N      | 2.47                     | 0.47              |
| 5:XE:8:GLU:OE2     | 5:XE:63:ARG:NH2   | 2.46                     | 0.47              |
| 8:XH:49:GLU:HG2    | 8:XH:62:TYR:HE2   | 1.78                     | 0.47              |
| 10:XJ:38:ILE:HD11  | 10:XJ:71:LEU:HD23 | 1.96                     | 0.47              |
| 18:XR:36:ASN:ND2   | 18:XR:36:ASN:O    | 2.41                     | 0.47              |
| 22:XV:5:G:H1       | 22:XV:67:C:H42    | 1.62                     | 0.47              |
| 25:YA:593:G:O4'    | 54:Y8:4:MET:HE1   | 2.13                     | 0.47              |
| 25:YA:1103:A:H5'   | 25:YA:1104:C:H5   | 1.79                     | 0.47              |
| 25:YA:1013:C:N4    | 25:YA:1149:G:H1   | 2.11                     | 0.47              |
| 25:YA:2511:U:O4    | 25:YA:2575:C:N3   | 2.46                     | 0.47              |
| 25:YA:807:U:H2'    | 25:YA:808:G:H8    | 1.78                     | 0.47              |
| 25:YA:99:U:H1'     | 25:YA:101:G:OP2   | 2.14                     | 0.47              |
| 31:YH:6:ARG:HA     | 31:YH:66:GLY:HA2  | 1.95                     | 0.47              |
| 1:QA:784:C:H4'     | 25:RA:1837:C:OP1  | 2.14                     | 0.47              |
| 2:QB:70:PHE:O      | 2:QB:93:VAL:N     | 2.48                     | 0.47              |
| 4:QD:12:CYS:HA     | 4:QD:19:LEU:CD2   | 2.45                     | 0.47              |
| 6:QF:41:GLU:HB2    | 6:QF:62:TRP:CE3   | 2.50                     | 0.47              |
| 12:QL:102:ARG:HB3  | 12:QL:102:ARG:HE  | 1.39                     | 0.47              |
| 17:QQ:100:LYS:O    | 17:QQ:101:ARG:NE  | 2.47                     | 0.47              |
| 20:QT:30:LYS:O     | 20:QT:33:ILE:HB   | 2.14                     | 0.47              |
| 47:R1:91:LYS:O     | 47:R1:94:LEU:N    | 2.36                     | 0.47              |
| 55:R9:27:CYS:SG    | 55:R9:32:HIS:HB2  | 2.55                     | 0.47              |
| 25:RA:2328:A:H2'   | 25:RA:2329:G:C8   | 2.49                     | 0.47              |
| 25:RA:99:U:H4'     | 25:RA:101:G:O5'   | 2.14                     | 0.47              |
| 36:RQ:136:ALA:C    | 36:RQ:138:ASP:H   | 2.18                     | 0.47              |
| 39:RT:64:ARG:HD2   | 39:RT:73:GLU:OE1  | 2.14                     | 0.47              |
| 25:RA:1754:C:P     | 39:RT:96:ARG:HH12 | 2.37                     | 0.47              |
| 1:XA:1308:U:H2'    | 1:XA:1309:G:H8    | 1.77                     | 0.47              |
| 2:XB:84:GLU:OE1    | 2:XB:87:ARG:NH2   | 2.43                     | 0.47              |
| 3:XC:34:LEU:HD23   | 3:XC:38:ARG:HG3   | 1.95                     | 0.47              |
| 3:XC:81:GLY:O      | 3:XC:85:ARG:HB2   | 2.14                     | 0.47              |
| 4:XD:15:GLU:HG2    | 4:XD:63:LYS:HB2   | 1.97                     | 0.47              |
| 6:XF:69:GLU:O      | 6:XF:72:VAL:HG12  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:XI:121:ARG:NH1  | 9:XI:122:ALA:O    | 2.47                     | 0.47              |
| 1:XA:539:A:OP2    | 12:XL:115:LYS:HE3 | 2.13                     | 0.47              |
| 18:XR:66:LEU:O    | 18:XR:70:ILE:HG13 | 2.14                     | 0.47              |
| 47:Y1:91:LYS:HB3  | 47:Y1:92:LYS:H    | 1.44                     | 0.47              |
| 25:YA:72:U:N3     | 48:Y2:62:THR:HG22 | 2.30                     | 0.47              |
| 25:YA:2210:G:H5'  | 25:YA:2211:G:C5   | 2.49                     | 0.47              |
| 25:YA:2590:A:OP2  | 27:YD:238:GLY:HA2 | 2.15                     | 0.47              |
| 36:YQ:21:THR:HB   | 36:YQ:22:LYS:H    | 1.40                     | 0.47              |
| 1:QA:1213:A:N1    | 1:QA:1215:G:H1'   | 2.30                     | 0.47              |
| 1:QA:1226:C:H2'   | 13:QM:103:THR:HB  | 1.95                     | 0.47              |
| 1:QA:321:A:N6     | 1:QA:329:A:OP2    | 2.48                     | 0.47              |
| 4:QD:26:CYS:HA    | 4:QD:31:CYS:HA    | 1.96                     | 0.47              |
| 17:QQ:76:LEU:HD21 | 17:QQ:79:SER:HB2  | 1.97                     | 0.47              |
| 22:QV:53:G:HO2'   | 22:QV:54:U:H5     | 1.62                     | 0.47              |
| 30:RG:3:LEU:HD11  | 50:R4:25:TYR:CE1  | 2.48                     | 0.47              |
| 51:R5:56:LYS:HB2  | 51:R5:58:LEU:HG   | 1.96                     | 0.47              |
| 25:RA:1028:A:N6   | 25:RA:1125:G:H2'  | 2.29                     | 0.47              |
| 25:RA:1794:U:H2'  | 25:RA:1795:C:C6   | 2.49                     | 0.47              |
| 25:RA:205:G:H1'   | 25:RA:206:U:OP2   | 2.14                     | 0.47              |
| 25:RA:611:C:H2'   | 25:RA:612:G:H8    | 1.80                     | 0.47              |
| 28:RE:21:VAL:CG2  | 28:RE:22:PRO:N    | 2.74                     | 0.47              |
| 29:RF:6:VAL:CG1   | 29:RF:24:LEU:HD23 | 2.43                     | 0.47              |
| 32:RI:55:ALA:HA   | 32:RI:58:LEU:HB2  | 1.94                     | 0.47              |
| 25:RA:1952:A:C2   | 34:RO:22:ILE:HG23 | 2.50                     | 0.47              |
| 40:RU:97:ASP:OD2  | 40:RU:101:ARG:NH1 | 2.48                     | 0.47              |
| 1:XA:532:A:H2     | 1:XA:1206:G:H21   | 1.63                     | 0.47              |
| 1:XA:627:G:H2'    | 1:XA:628:G:C8     | 2.50                     | 0.47              |
| 1:XA:695:A:H61    | 1:XA:797:C:H1'    | 1.78                     | 0.47              |
| 3:XC:22:TRP:CD1   | 3:XC:59:ARG:HD2   | 2.49                     | 0.47              |
| 3:XC:79:ARG:NH1   | 3:XC:82:GLU:HG3   | 2.29                     | 0.47              |
| 9:XI:126:SER:O    | 9:XI:128:ARG:N    | 2.43                     | 0.47              |
| 1:XA:963:G:H21    | 10:XJ:55:LYS:CE   | 2.27                     | 0.47              |
| 22:XV:15:C:H5''   | 22:XV:16:C:H5     | 1.79                     | 0.47              |
| 48:Y2:59:ARG:O    | 48:Y2:63:VAL:HG23 | 2.15                     | 0.47              |
| 54:Y8:36:LYS:HB3  | 54:Y8:40:GLU:HG2  | 1.95                     | 0.47              |
| 25:YA:242:G:H4'   | 25:YA:243:U:O5'   | 2.14                     | 0.47              |
| 25:YA:2789:C:H1'  | 25:YA:2892:A:C2   | 2.46                     | 0.47              |
| 25:YA:740:U:H5''  | 25:YA:1784:A:H3'  | 1.95                     | 0.47              |
| 25:YA:764:A:H5'   | 27:YD:210:GLY:HA2 | 1.95                     | 0.47              |
| 27:YD:71:ASP:HB2  | 27:YD:103:ARG:NH2 | 2.27                     | 0.47              |
| 35:YP:144:GLU:N   | 35:YP:144:GLU:OE1 | 2.40                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1321:C:H5''  | 1:QA:1322:C:H5''   | 1.97                     | 0.47              |
| 1:QA:1443:G:H5'   | 1:QA:1446:A:OP2    | 2.15                     | 0.47              |
| 1:QA:1513:A:H2'   | 1:QA:1514:C:C6     | 2.50                     | 0.47              |
| 1:QA:377:G:H1     | 1:QA:386:C:H42     | 1.61                     | 0.47              |
| 2:QB:211:ILE:O    | 2:QB:215:LEU:HB2   | 2.14                     | 0.47              |
| 2:QB:25:ASN:O     | 2:QB:27:LYS:N      | 2.47                     | 0.47              |
| 12:QL:51:ALA:HB3  | 12:QL:53:ARG:HE    | 1.80                     | 0.47              |
| 14:QN:41:ARG:CZ   | 14:QN:42:ILE:HD11  | 2.44                     | 0.47              |
| 22:QV:16:C:N4     | 22:QV:17:U:O4      | 2.48                     | 0.47              |
| 25:RA:686:G:H8    | 53:R7:6:GLN:O      | 1.97                     | 0.47              |
| 25:RA:2058:A:C2   | 56:Z7:1:T17:O48    | 2.66                     | 0.47              |
| 25:RA:2327:A:H2'  | 25:RA:2328:A:C8    | 2.49                     | 0.47              |
| 25:RA:2823:A:OP1  | 28:RE:113:PHE:HB2  | 2.15                     | 0.47              |
| 25:RA:581:C:H2'   | 25:RA:582:G:H8     | 1.78                     | 0.47              |
| 28:RE:37:ARG:HA   | 28:RE:37:ARG:NE    | 2.29                     | 0.47              |
| 25:RA:662:G:H5'   | 35:RP:15:ARG:HA    | 1.95                     | 0.47              |
| 36:RQ:63:LYS:HG2  | 36:RQ:65:PHE:CE1   | 2.50                     | 0.47              |
| 44:RY:21:LYS:HG3  | 44:RY:22:GLY:N     | 2.30                     | 0.47              |
| 1:XA:619:U:H3     | 4:XD:135:LEU:HD23  | 1.80                     | 0.47              |
| 15:XO:66:LEU:HD12 | 15:XO:66:LEU:HA    | 1.67                     | 0.47              |
| 20:XT:35:THR:O    | 20:XT:39:LYS:HG3   | 2.14                     | 0.47              |
| 25:YA:2154:G:H2'  | 25:YA:2155:G:C8    | 2.48                     | 0.47              |
| 31:YH:153:LYS:HB3 | 31:YH:154:PRO:HD3  | 1.96                     | 0.47              |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:H    | 1.80                     | 0.47              |
| 1:QA:1414:U:H2'   | 1:QA:1415:G:H8     | 1.80                     | 0.47              |
| 9:QL:28:VAL:HG22  | 9:QL:63:ILE:HB     | 1.95                     | 0.47              |
| 10:QJ:61:GLU:HG3  | 14:QN:58:LYS:HZ1   | 1.79                     | 0.47              |
| 12:QL:27:LEU:O    | 12:QL:29:GLY:N     | 2.47                     | 0.47              |
| 25:RA:1407:C:H42  | 25:RA:1595:G:H1    | 1.62                     | 0.47              |
| 25:RA:1667:G:O2'  | 25:RA:1991:U:O4    | 2.32                     | 0.47              |
| 25:RA:2747:G:N2   | 25:RA:2757:A:H62   | 2.11                     | 0.47              |
| 25:RA:706:A:H2'   | 25:RA:707:G:O4'    | 2.14                     | 0.47              |
| 32:RI:98:ALA:HA   | 32:RI:109:ILE:HD11 | 1.97                     | 0.47              |
| 42:RW:63:ASP:OD1  | 42:RW:63:ASP:N     | 2.48                     | 0.47              |
| 1:XA:1237:C:O2'   | 1:XA:1300:G:N2     | 2.44                     | 0.47              |
| 1:XA:1305:G:H1'   | 1:XA:1332:A:N6     | 2.29                     | 0.47              |
| 1:XA:1469:G:H2'   | 1:XA:1470:G:C8     | 2.50                     | 0.47              |
| 2:XB:93:VAL:HG11  | 2:XB:97:TRP:CD1    | 2.50                     | 0.47              |
| 9:XI:4:TYR:CZ     | 9:XI:88:TYR:HB2    | 2.49                     | 0.47              |
| 10:XJ:47:PHE:HB3  | 14:YN:34:TYR:CE2   | 2.50                     | 0.47              |
| 12:XL:24:VAL:HG12 | 12:XL:24:VAL:O     | 2.14                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:XM:53:VAL:HG12  | 13:XM:57:ARG:NH1  | 2.27                     | 0.47              |
| 46:Y0:19:LYS:HA    | 46:Y0:19:LYS:HD3  | 1.66                     | 0.47              |
| 47:Y1:53:VAL:HG22  | 47:Y1:74:VAL:HG13 | 1.96                     | 0.47              |
| 25:YA:2182:G:H2'   | 25:YA:2183:C:C6   | 2.50                     | 0.47              |
| 25:YA:2287:A:N6    | 25:YA:2344:U:C2   | 2.83                     | 0.47              |
| 25:YA:2732:G:H3'   | 25:YA:2733:A:O4'  | 2.14                     | 0.47              |
| 25:YA:479:A:N3     | 25:YA:481:G:H5''  | 2.30                     | 0.47              |
| 25:YA:498:G:H1'    | 44:YY:47:LYS:HZ3  | 1.79                     | 0.47              |
| 26:YB:37:C:N3      | 26:YB:48:A:O2'    | 2.41                     | 0.47              |
| 29:YF:164:ARG:HG3  | 29:YF:175:THR:OG1 | 2.15                     | 0.47              |
| 39:YT:11:GLU:N     | 39:YT:11:GLU:OE1  | 2.43                     | 0.47              |
| 25:YA:137(A):G:H1' | 43:YX:41:ASN:HD22 | 1.76                     | 0.47              |
| 44:YY:73:ARG:HB3   | 44:YY:73:ARG:HE   | 1.47                     | 0.47              |
| 45:YZ:182:LYS:CG   | 45:YZ:183:LEU:HA  | 2.44                     | 0.47              |
| 1:QA:1084:G:H5'    | 1:QA:1102:A:OP2   | 2.14                     | 0.47              |
| 1:QA:1126:U:H1'    | 1:QA:1280:A:C5    | 2.49                     | 0.47              |
| 1:QA:713:G:H2'     | 1:QA:714:G:C8     | 2.49                     | 0.47              |
| 1:QA:1128:C:C4'    | 9:QI:16:ARG:HH22  | 2.28                     | 0.47              |
| 12:QL:17:LYS:HG3   | 12:QL:18:VAL:N    | 2.30                     | 0.47              |
| 13:QM:78:ILE:HG23  | 13:QM:92:HIS:ND1  | 2.29                     | 0.47              |
| 1:QA:273:A:H1'     | 17:QQ:16:GLN:OE1  | 2.15                     | 0.47              |
| 22:QV:21:A:N6      | 22:QV:46:G:H2'    | 2.30                     | 0.47              |
| 19:QS:67:VAL:N     | 50:R4:59:PHE:HZ   | 2.08                     | 0.47              |
| 25:RA:2086:U:H2'   | 25:RA:2087:G:C8   | 2.49                     | 0.47              |
| 25:RA:2512:C:H2'   | 25:RA:2513:G:O4'  | 2.14                     | 0.47              |
| 25:RA:2698:U:H2'   | 25:RA:2699:C:C6   | 2.49                     | 0.47              |
| 25:RA:740:U:H2'    | 25:RA:741:G:C8    | 2.50                     | 0.47              |
| 28:RE:73:GLU:HG3   | 28:RE:74:PRO:HD2  | 1.95                     | 0.47              |
| 1:XA:377:G:P       | 16:XP:5:ARG:HH11  | 2.37                     | 0.47              |
| 9:XI:114:TYR:HD2   | 10:XJ:60:ARG:HB2  | 1.79                     | 0.47              |
| 19:XS:68:GLY:CA    | 50:Y4:59:PHE:CE1  | 2.86                     | 0.47              |
| 25:YA:26:G:H1'     | 25:YA:515:A:H61   | 1.79                     | 0.47              |
| 30:YG:28:VAL:O     | 30:YG:31:VAL:HG13 | 2.14                     | 0.47              |
| 33:YN:30:ILE:HG22  | 33:YN:34:LEU:HD22 | 1.96                     | 0.47              |
| 25:YA:1454:U:H5'   | 37:YR:63:ARG:HE   | 1.79                     | 0.47              |
| 1:QA:265:G:H2'     | 1:QA:266:G:H5''   | 1.97                     | 0.47              |
| 4:QD:30:LYS:N      | 4:QD:30:LYS:CD    | 2.77                     | 0.47              |
| 6:QF:61:LEU:HB3    | 6:QF:63:TYR:HE1   | 1.80                     | 0.47              |
| 25:RA:576:U:OP1    | 25:RA:2503:A:OP1  | 2.33                     | 0.47              |
| 25:RA:2849:U:H4'   | 25:RA:2868:A:C2   | 2.50                     | 0.47              |
| 25:RA:764:A:H5'    | 27:RD:210:GLY:HA2 | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:152:ARG:HG3  | 31:RH:153:LYS:CD   | 2.44                     | 0.47              |
| 32:RI:88:ILE:HG12  | 32:RI:122:GLU:H    | 1.80                     | 0.47              |
| 37:RR:1:MET:HB3    | 37:RR:2:ARG:H      | 1.35                     | 0.47              |
| 39:RT:123:GLN:O    | 39:RT:125:ARG:N    | 2.48                     | 0.47              |
| 45:RZ:141:VAL:HA   | 45:RZ:144:LEU:HD23 | 1.96                     | 0.47              |
| 1:XA:1308:U:H2'    | 1:XA:1309:G:C8     | 2.49                     | 0.47              |
| 1:XA:244:U:H4'     | 1:XA:245:C:O5'     | 2.14                     | 0.47              |
| 1:XA:28:G:H1       | 1:XA:555:C:H42     | 1.61                     | 0.47              |
| 1:XA:327:A:O2'     | 1:XA:328:C:O4'     | 2.29                     | 0.47              |
| 1:XA:345:C:H4'     | 1:XA:346:G:O5'     | 2.15                     | 0.47              |
| 2:XB:18:GLY:H      | 2:XB:42:ILE:HG22   | 1.80                     | 0.47              |
| 11:XK:48:ILE:HG13  | 11:XK:63:LEU:HB2   | 1.97                     | 0.47              |
| 23:XW:39:U:H4'     | 23:XW:39:U:OP1     | 2.14                     | 0.47              |
| 25:YA:2372:G:O2'   | 52:Y6:46:HIS:NE2   | 2.27                     | 0.47              |
| 25:YA:2308:G:N1    | 25:YA:2311:A:C2    | 2.61                     | 0.47              |
| 25:YA:2867:G:O2'   | 25:YA:2868:A:P     | 2.73                     | 0.47              |
| 25:YA:372:G:H1'    | 25:YA:373:U:H5     | 1.80                     | 0.47              |
| 27:YD:237:GLU:O    | 27:YD:239:ARG:N    | 2.47                     | 0.47              |
| 29:YF:129:PHE:HA   | 29:YF:142:TRP:NE1  | 2.29                     | 0.47              |
| 29:YF:182:ASN:HD21 | 29:YF:185:ASP:CG   | 2.14                     | 0.47              |
| 30:YG:113:ARG:HG2  | 50:Y4:34:GLU:OE2   | 2.14                     | 0.47              |
| 30:YG:34:LEU:HD22  | 30:YG:35:GLU:N     | 2.30                     | 0.47              |
| 1:QA:1301:U:O2     | 1:QA:1301:U:H2'    | 2.13                     | 0.47              |
| 1:QA:1515:C:H2'    | 1:QA:1516:G:C8     | 2.50                     | 0.47              |
| 1:QA:34:C:H2'      | 1:QA:35:G:C8       | 2.50                     | 0.47              |
| 1:QA:736:C:H2'     | 1:QA:737:A:C8      | 2.49                     | 0.47              |
| 2:QB:8:LYS:HD3     | 2:QB:8:LYS:H       | 1.79                     | 0.47              |
| 7:QG:99:LEU:HD22   | 7:QG:103:TRP:CZ2   | 2.49                     | 0.47              |
| 1:QA:690:G:H22     | 11:QK:55:LYS:HZ2   | 1.62                     | 0.47              |
| 25:RA:1292:U:H2'   | 25:RA:1293:C:C6    | 2.50                     | 0.47              |
| 25:RA:1348:G:H2'   | 25:RA:1349:A:H5''  | 1.97                     | 0.47              |
| 25:RA:2150:U:H2'   | 25:RA:2151:G:C8    | 2.50                     | 0.47              |
| 25:RA:2116:G:H1    | 25:RA:2162:G:P     | 2.38                     | 0.47              |
| 25:RA:2689:U:H4'   | 25:RA:2690:C:O5'   | 2.13                     | 0.47              |
| 25:RA:2779:U:O2'   | 25:RA:2781:A:C5    | 2.66                     | 0.47              |
| 25:RA:389:G:N1     | 35:RP:70:GLN:HB3   | 2.30                     | 0.47              |
| 25:RA:628:G:O2'    | 25:RA:651:G:O2'    | 2.17                     | 0.47              |
| 28:RE:95:ILE:HD12  | 28:RE:95:ILE:H     | 1.80                     | 0.47              |
| 29:RF:133:ASN:HA   | 29:RF:162:LEU:HD22 | 1.96                     | 0.47              |
| 29:RF:62:ARG:HB3   | 29:RF:62:ARG:CZ    | 2.45                     | 0.47              |
| 31:RH:27:LYS:HA    | 31:RH:32:GLU:HA    | 1.96                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:HH22  | 1.80                     | 0.47              |
| 44:RY:76:CYS:HB2    | 44:RY:101:LYS:HG3  | 1.96                     | 0.47              |
| 1:XA:900:A:H2'      | 1:XA:901:A:C8      | 2.49                     | 0.47              |
| 12:XL:46:LYS:CG     | 12:XL:47:LYS:H     | 2.27                     | 0.47              |
| 17:XQ:67:LYS:O      | 17:XQ:68:ARG:HB3   | 2.15                     | 0.47              |
| 23:XW:21:A:N6       | 23:XW:46:G:N3      | 2.63                     | 0.47              |
| 25:YA:1316:U:H2'    | 25:YA:1317:A:H8    | 1.79                     | 0.47              |
| 25:YA:587:C:N3      | 35:YP:33:ARG:NH1   | 2.62                     | 0.47              |
| 25:YA:443:A:N7      | 29:YF:45:ARG:HD2   | 2.30                     | 0.47              |
| 30:YG:114:ILE:HD13  | 30:YG:140:ILE:HG21 | 1.96                     | 0.47              |
| 31:YH:122:THR:HG22  | 31:YH:134:SER:HB2  | 1.96                     | 0.47              |
| 31:YH:4:ILE:HG13    | 31:YH:6:ARG:CZ     | 2.44                     | 0.47              |
| 31:YH:4:ILE:HB      | 31:YH:6:ARG:CG     | 2.43                     | 0.47              |
| 35:YP:19:VAL:HG13   | 35:YP:21:ARG:N     | 2.20                     | 0.47              |
| 36:YQ:81:VAL:O      | 36:YQ:82:ARG:NE    | 2.48                     | 0.47              |
| 25:YA:896:A:H61     | 45:YZ:112:ARG:NH1  | 2.12                     | 0.47              |
| 1:QA:1200:C:H4'     | 1:QA:1201:A:H5'    | 1.96                     | 0.47              |
| 1:QA:1443:G:N2      | 39:RT:119:LYS:HB2  | 2.30                     | 0.47              |
| 1:QA:671:G:H1       | 1:QA:735:C:H42     | 1.62                     | 0.47              |
| 7:QG:18:TYR:HD2     | 7:QG:59:LEU:HD22   | 1.79                     | 0.47              |
| 19:QS:15:LEU:H      | 19:QS:15:LEU:HD23  | 1.79                     | 0.47              |
| 23:QW:30:G:H2'      | 23:QW:31:A:C8      | 2.49                     | 0.47              |
| 47:R1:76:ARG:H      | 47:R1:76:ARG:HD2   | 1.80                     | 0.47              |
| 25:RA:2735:G:H2'    | 25:RA:2736:G:C8    | 2.48                     | 0.47              |
| 25:RA:389:G:H1      | 35:RP:70:GLN:HB3   | 1.79                     | 0.47              |
| 25:RA:709:U:H2'     | 25:RA:710:G:C8     | 2.50                     | 0.47              |
| 26:RB:8:U:O3'       | 38:RS:25:ARG:NH2   | 2.47                     | 0.47              |
| 38:RS:56:LEU:O      | 38:RS:58:LEU:N     | 2.48                     | 0.47              |
| 41:RV:24:LYS:HG3    | 41:RV:92:THR:HG23  | 1.97                     | 0.47              |
| 43:RX:49:VAL:HG13   | 43:RX:83:VAL:HG13  | 1.96                     | 0.47              |
| 17:XQ:63:ARG:HG2    | 17:XQ:64:PRO:HD2   | 1.97                     | 0.47              |
| 9:XI:128:ARG:NH1    | 22:XV:33:U:OP2     | 2.28                     | 0.47              |
| 23:XW:16:U:C5       | 23:XW:18:G:H3'     | 2.50                     | 0.47              |
| 25:YA:577:G:O2'     | 25:YA:1254:A:OP1   | 2.29                     | 0.47              |
| 25:YA:1360:A:C6     | 25:YA:1372:U:C4    | 3.03                     | 0.47              |
| 25:YA:1697:G:H5''   | 25:YA:1698:A:H3'   | 1.96                     | 0.47              |
| 29:YF:9:ILE:HG23    | 29:YF:20:LEU:O     | 2.15                     | 0.47              |
| 38:YS:52:SER:HB2    | 38:YS:55:ALA:H     | 1.80                     | 0.47              |
| 1:QA:452:A:O2'      | 1:QA:453:A:O4'     | 2.30                     | 0.47              |
| 1:QA:962:C:H42      | 1:QA:974:A:H61     | 1.62                     | 0.47              |
| 2:QB:32:ILE:HD13    | 2:QB:40:HIS:HB3    | 1.95                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:QE:9:LYS:HB3     | 5:QE:112:LEU:HD11 | 1.97                     | 0.47              |
| 19:QS:35:SER:O     | 19:QS:71:LEU:HD12 | 2.15                     | 0.47              |
| 51:R5:52:TYR:O     | 51:R5:53:ALA:HB3  | 2.14                     | 0.47              |
| 25:RA:117:G:OP2    | 25:RA:119:A:O2'   | 2.22                     | 0.47              |
| 25:RA:1359:A:C6    | 25:RA:1373:A:C5   | 3.03                     | 0.47              |
| 25:RA:2378:A:O5'   | 25:RA:2378:A:H8   | 1.99                     | 0.47              |
| 25:RA:2387:U:O2'   | 46:R0:19:LYS:NZ   | 2.48                     | 0.47              |
| 25:RA:2610:C:H4'   | 25:RA:2611:U:OP2  | 2.14                     | 0.47              |
| 25:RA:2645:G:C3'   | 25:RA:2646:C:H5'  | 2.45                     | 0.47              |
| 25:RA:2867:G:O2'   | 25:RA:2868:A:P    | 2.73                     | 0.47              |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:N   | 2.29                     | 0.47              |
| 27:RD:211:ARG:HD2  | 27:RD:214:TRP:CZ3 | 2.50                     | 0.47              |
| 32:RI:9:LEU:O      | 32:RI:10:GLU:HG3  | 2.15                     | 0.47              |
| 38:RS:48:LEU:HD23  | 38:RS:82:ILE:HD11 | 1.96                     | 0.47              |
| 1:XA:1126:U:H1'    | 1:XA:1280:A:C5    | 2.50                     | 0.47              |
| 1:XA:1159:U:O2'    | 1:XA:1160:G:N7    | 2.44                     | 0.47              |
| 1:XA:210:U:O2'     | 1:XA:216:G:N7     | 2.45                     | 0.47              |
| 50:Y4:38:LYS:HD3   | 50:Y4:42:PHE:HE1  | 1.80                     | 0.47              |
| 25:YA:1472:A:H2'   | 25:YA:1473:G:O4'  | 2.15                     | 0.47              |
| 25:YA:2243:U:H2'   | 25:YA:2244:U:C6   | 2.50                     | 0.47              |
| 25:YA:2401:U:H2'   | 25:YA:2402:C:H5'' | 1.97                     | 0.47              |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:C8 | 2.50                     | 0.47              |
| 27:YD:17:THR:CG2   | 27:YD:205:VAL:H   | 2.28                     | 0.47              |
| 28:YE:116:VAL:HG11 | 28:YE:138:PRO:HB3 | 1.97                     | 0.47              |
| 28:YE:150:VAL:HG13 | 28:YE:154:LYS:HG3 | 1.96                     | 0.47              |
| 30:YG:11:TYR:HA    | 30:YG:15:VAL:HB   | 1.95                     | 0.47              |
| 32:YI:144:VAL:HG22 | 32:YI:145:VAL:H   | 1.80                     | 0.47              |
| 35:YP:29:LYS:HD2   | 35:YP:30:THR:HG23 | 1.97                     | 0.47              |
| 1:QA:606:G:H22     | 1:QA:631:G:H5'    | 1.80                     | 0.46              |
| 1:QA:953:G:C5'     | 1:QA:965:A:H61    | 2.27                     | 0.46              |
| 3:QC:82:GLU:O      | 3:QC:86:VAL:HG13  | 2.14                     | 0.46              |
| 10:QJ:84:GLN:HG3   | 10:QJ:84:GLN:H    | 1.49                     | 0.46              |
| 54:R8:29:LYS:HD3   | 54:R8:44:LYS:CB   | 2.45                     | 0.46              |
| 25:RA:1287:A:N7    | 37:RR:107:ASP:HB2 | 2.30                     | 0.46              |
| 25:RA:1796:U:H2'   | 25:RA:1797:C:C6   | 2.50                     | 0.46              |
| 25:RA:2562:U:O2'   | 34:RO:23:ARG:NH1  | 2.44                     | 0.46              |
| 25:RA:50:U:H3'     | 25:RA:51:G:H5'    | 1.97                     | 0.46              |
| 25:RA:639:U:H2'    | 25:RA:640:C:C6    | 2.49                     | 0.46              |
| 26:RB:16:G:H1      | 26:RB:68:C:N4     | 2.13                     | 0.46              |
| 27:RD:12:SER:O     | 27:RD:16:MET:HB2  | 2.14                     | 0.46              |
| 27:RD:43:ARG:HH11  | 27:RD:44:ASN:CG   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:RP:83:VAL:HG12 | 35:RP:114:ILE:HA   | 1.97                     | 0.46              |
| 39:RT:20:PRO:HD2  | 39:RT:86:ILE:HG23  | 1.97                     | 0.46              |
| 1:XA:1125:U:OP2   | 1:XA:1145:C:N4     | 2.48                     | 0.46              |
| 1:XA:1315:U:H2'   | 1:XA:1316:G:O4'    | 2.15                     | 0.46              |
| 1:XA:565:U:H5''   | 1:XA:566:G:H2'     | 1.97                     | 0.46              |
| 1:XA:93:U:H2'     | 1:XA:95:G:O4'      | 2.15                     | 0.46              |
| 2:XB:201:ILE:HG21 | 2:XB:214:ILE:HG21  | 1.95                     | 0.46              |
| 3:XC:14:ILE:HG12  | 3:XC:15:THR:N      | 2.30                     | 0.46              |
| 5:XE:89:ILE:HG12  | 5:XE:91:LEU:HD13   | 1.97                     | 0.46              |
| 12:XL:47:LYS:CB   | 12:XL:48:PRO:CD    | 2.92                     | 0.46              |
| 1:XA:735:C:H5'    | 18:XR:71:LYS:HD3   | 1.96                     | 0.46              |
| 19:XS:33:THR:OG1  | 19:XS:34:TRP:N     | 2.49                     | 0.46              |
| 19:XS:41:VAL:HA   | 19:XS:44:MET:HG3   | 1.97                     | 0.46              |
| 49:Y3:23:LEU:HD13 | 49:Y3:50:VAL:HG11  | 1.96                     | 0.46              |
| 25:YA:2527:C:H5'' | 55:Y9:30:PRO:HB2   | 1.96                     | 0.46              |
| 29:YF:108:LYS:NZ  | 29:YF:108:LYS:HB3  | 2.31                     | 0.46              |
| 35:YP:88:LEU:HB2  | 35:YP:91:PHE:HE1   | 1.80                     | 0.46              |
| 38:YS:27:SER:HA   | 38:YS:88:ASP:HB2   | 1.96                     | 0.46              |
| 44:YY:87:LYS:HD3  | 44:YY:92:ASN:HB3   | 1.98                     | 0.46              |
| 1:QA:1305:G:HO2'  | 1:QA:1306:A:H8     | 1.60                     | 0.46              |
| 1:QA:1306:A:N6    | 1:QA:1331:G:H1'    | 2.31                     | 0.46              |
| 1:QA:318:G:H2'    | 1:QA:319:G:H8      | 1.78                     | 0.46              |
| 7:QG:78:ARG:HG3   | 7:QG:79:ARG:N      | 2.30                     | 0.46              |
| 11:QK:16:SER:OG   | 11:QK:106:LYS:NZ   | 2.48                     | 0.46              |
| 13:QM:3:ARG:HH21  | 30:RG:139:LEU:HD13 | 1.79                     | 0.46              |
| 25:RA:2294:C:H2'  | 25:RA:2295:C:C6    | 2.50                     | 0.46              |
| 28:RE:186:GLY:O   | 28:RE:188:VAL:N    | 2.48                     | 0.46              |
| 25:RA:2444:G:P    | 29:RF:68:LYS:HE3   | 2.55                     | 0.46              |
| 29:RF:6:VAL:HG11  | 29:RF:24:LEU:HD23  | 1.97                     | 0.46              |
| 31:RH:153:LYS:HB3 | 31:RH:162:ILE:H    | 1.80                     | 0.46              |
| 32:RI:40:THR:O    | 32:RI:44:LEU:N     | 2.44                     | 0.46              |
| 39:RT:16:ARG:HE   | 39:RT:19:LEU:HD21  | 1.80                     | 0.46              |
| 40:RU:8:VAL:HG23  | 40:RU:11:ARG:HH21  | 1.80                     | 0.46              |
| 42:RW:23:LEU:O    | 42:RW:27:LYS:HD2   | 2.14                     | 0.46              |
| 44:RY:89:PHE:O    | 44:RY:90:LEU:HD13  | 2.15                     | 0.46              |
| 1:XA:511:C:HO2'   | 1:XA:512:U:H6      | 1.62                     | 0.46              |
| 4:XD:63:LYS:HD2   | 4:XD:198:VAL:HG22  | 1.97                     | 0.46              |
| 23:XY:37:A:H3'    | 23:XY:38:A:H8      | 1.80                     | 0.46              |
| 25:YA:1035:U:H2'  | 25:YA:1036:G:C8    | 2.50                     | 0.46              |
| 25:YA:1270:C:H5'' | 25:YA:1271:G:H5'   | 1.97                     | 0.46              |
| 25:YA:1434:A:H61  | 25:YA:1558:A:H62   | 1.62                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1639:U:H2'  | 25:YA:1640:C:H5''  | 1.96                     | 0.46              |
| 25:YA:1796:U:H2'  | 25:YA:1797:C:C6    | 2.49                     | 0.46              |
| 25:YA:2031:A:N3   | 25:YA:2455:G:O2'   | 2.39                     | 0.46              |
| 25:YA:2277:G:OP2  | 46:Y0:10:THR:HG21  | 2.15                     | 0.46              |
| 25:YA:2543:G:H2'  | 25:YA:2544:G:C8    | 2.49                     | 0.46              |
| 25:YA:2728:U:H2'  | 25:YA:2729:G:C8    | 2.51                     | 0.46              |
| 25:YA:957:A:N1    | 25:YA:2458:G:H4'   | 2.30                     | 0.46              |
| 29:YF:127:GLU:OE2 | 29:YF:128:ALA:N    | 2.47                     | 0.46              |
| 32:YI:68:LEU:HA   | 32:YI:71:ILE:HG22  | 1.97                     | 0.46              |
| 35:YP:96:THR:O    | 35:YP:99:LEU:HB3   | 2.15                     | 0.46              |
| 1:QA:1376:U:H2'   | 1:QA:1377:A:C8     | 2.50                     | 0.46              |
| 1:QA:224:C:H2'    | 1:QA:225:C:C6      | 2.51                     | 0.46              |
| 1:QA:403:C:H2'    | 1:QA:404:U:H6      | 1.81                     | 0.46              |
| 1:QA:932:C:H4'    | 7:QG:4:ARG:NH2     | 2.30                     | 0.46              |
| 25:RA:2271:G:OP1  | 46:R0:18:ALA:HB1   | 2.15                     | 0.46              |
| 47:R1:89:GLU:HA   | 47:R1:93:GLU:HB2   | 1.96                     | 0.46              |
| 52:R6:13:CYS:HB2  | 52:R6:22:ALA:HB3   | 1.98                     | 0.46              |
| 25:RA:1007:C:OP1  | 33:RN:37:LYS:NZ    | 2.41                     | 0.46              |
| 25:RA:1278:A:H4'  | 37:RR:34:ILE:HD12  | 1.96                     | 0.46              |
| 25:RA:1801:G:OP2  | 27:RD:154:LYS:HE2  | 2.16                     | 0.46              |
| 25:RA:222:A:H3'   | 25:RA:421:U:H5''   | 1.96                     | 0.46              |
| 25:RA:2680:C:OP2  | 28:RE:111:ARG:NH2  | 2.48                     | 0.46              |
| 25:RA:2758:A:H2'  | 25:RA:2759:G:O4'   | 2.15                     | 0.46              |
| 27:RD:70:TRP:CD2  | 27:RD:150:LYS:HD2  | 2.49                     | 0.46              |
| 30:RG:22:ARG:HH22 | 30:RG:175:LEU:HD21 | 1.80                     | 0.46              |
| 32:RI:104:GLN:C   | 32:RI:105:HIS:HD1  | 2.18                     | 0.46              |
| 38:RS:78:LEU:HD11 | 38:RS:107:GLU:O    | 2.15                     | 0.46              |
| 3:XC:178:LEU:HD13 | 3:XC:178:LEU:HA    | 1.84                     | 0.46              |
| 1:XA:1314:C:N4    | 19:XS:2:PRO:O      | 2.48                     | 0.46              |
| 19:XS:41:VAL:HG23 | 19:XS:67:VAL:HG13  | 1.98                     | 0.46              |
| 46:Y0:17:GLN:O    | 46:Y0:19:LYS:HE3   | 2.14                     | 0.46              |
| 25:YA:1087:G:C5   | 25:YA:1089:G:H1'   | 2.50                     | 0.46              |
| 25:YA:407:G:H2'   | 25:YA:408:G:H8     | 1.80                     | 0.46              |
| 25:YA:483:A:H3'   | 25:YA:484:C:H6     | 1.81                     | 0.46              |
| 27:YD:94:LEU:HD22 | 27:YD:95:LEU:N     | 2.31                     | 0.46              |
| 33:YN:114:ARG:O   | 33:YN:115:ARG:HB3  | 2.15                     | 0.46              |
| 1:QA:22:G:H2'     | 1:QA:23:C:C6       | 2.50                     | 0.46              |
| 2:QB:166:ASP:OD2  | 2:QB:169:LYS:HB2   | 2.15                     | 0.46              |
| 1:QA:405:U:O4     | 4:QD:2:GLY:N       | 2.49                     | 0.46              |
| 19:QS:63:THR:HG23 | 19:QS:65:ASN:OD1   | 2.15                     | 0.46              |
| 25:RA:1936:A:H61  | 25:RA:1963:U:H3    | 1.63                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2623:G:OP1   | 25:RA:2826:A:O2'   | 2.22                     | 0.46              |
| 34:RO:76:ALA:HB3   | 39:RT:75:ILE:HB    | 1.97                     | 0.46              |
| 1:XA:673:G:H2'     | 1:XA:674:G:C8      | 2.50                     | 0.46              |
| 1:XA:689:C:H3'     | 1:XA:690:G:H21     | 1.80                     | 0.46              |
| 7:XG:115:ARG:HB2   | 7:XG:118:VAL:HG22  | 1.97                     | 0.46              |
| 7:XG:74:GLU:HG2    | 7:XG:91:VAL:HG22   | 1.98                     | 0.46              |
| 9:XI:18:PHE:HB2    | 9:XI:62:TYR:HB3    | 1.97                     | 0.46              |
| 9:XI:83:ARG:O      | 9:XI:86:VAL:HG12   | 2.15                     | 0.46              |
| 19:XS:41:VAL:HB    | 19:XS:42:PRO:HA    | 1.96                     | 0.46              |
| 20:XT:75:ASN:OD1   | 20:XT:75:ASN:N     | 2.40                     | 0.46              |
| 48:Y2:47:ASN:HB2   | 48:Y2:48:HIS:H     | 1.50                     | 0.46              |
| 49:Y3:8:LEU:HD22   | 49:Y3:31:LEU:HD22  | 1.96                     | 0.46              |
| 25:YA:1055:G:H1    | 25:YA:1104:C:N4    | 2.11                     | 0.46              |
| 25:YA:2334:G:C6    | 46:Y0:75:LEU:HD21  | 2.51                     | 0.46              |
| 26:YB:89(A):A:C5   | 26:YB:90:C:H1'     | 2.51                     | 0.46              |
| 27:YD:206:LEU:HA   | 27:YD:206:LEU:HD23 | 1.51                     | 0.46              |
| 27:YD:25:THR:CG2   | 27:YD:82:ILE:H     | 2.27                     | 0.46              |
| 28:YE:176:ILE:HB   | 28:YE:181:LEU:HB2  | 1.97                     | 0.46              |
| 35:YP:121:LYS:HE2  | 35:YP:121:LYS:HB2  | 1.74                     | 0.46              |
| 1:QA:1225:A:H5''   | 1:QA:1226:C:OP2    | 2.16                     | 0.46              |
| 1:QA:1298:C:H4'    | 1:QA:1299:A:C8     | 2.50                     | 0.46              |
| 1:QA:381:C:H2'     | 1:QA:382:A:O4'     | 2.14                     | 0.46              |
| 51:R5:56:LYS:HE2   | 51:R5:58:LEU:HD23  | 1.96                     | 0.46              |
| 25:RA:1678:G:N2    | 25:RA:1989:G:H22   | 2.13                     | 0.46              |
| 25:RA:581:C:H2'    | 25:RA:582:G:C8     | 2.50                     | 0.46              |
| 29:RF:126:VAL:HG11 | 29:RF:142:TRP:HH2  | 1.80                     | 0.46              |
| 35:RP:124:LYS:HA   | 35:RP:143:GLY:O    | 2.16                     | 0.46              |
| 43:RX:55:ASN:HB2   | 43:RX:80:ILE:HG23  | 1.97                     | 0.46              |
| 45:RZ:157:LEU:HA   | 45:RZ:158:PRO:HD2  | 1.70                     | 0.46              |
| 1:XA:1495:U:H2'    | 1:XA:1496:C:H6     | 1.81                     | 0.46              |
| 1:XA:954:G:N2      | 1:XA:1227:A:N6     | 2.52                     | 0.46              |
| 16:XP:1:MET:O      | 16:XP:3:LYS:HG3    | 2.15                     | 0.46              |
| 50:Y4:55:ARG:HG3   | 50:Y4:59:PHE:CD2   | 2.49                     | 0.46              |
| 25:YA:1113:U:H2'   | 25:YA:1114:G:C8    | 2.50                     | 0.46              |
| 25:YA:1579:A:H2'   | 25:YA:1580:A:C8    | 2.50                     | 0.46              |
| 25:YA:2324:C:H5''  | 25:YA:2325:G:H5'   | 1.97                     | 0.46              |
| 25:YA:304:G:H2'    | 25:YA:305:U:C6     | 2.51                     | 0.46              |
| 28:YE:36:ARG:NH2   | 28:YE:88:GLY:HA2   | 2.29                     | 0.46              |
| 31:YH:16:SER:O     | 31:YH:26:VAL:O     | 2.33                     | 0.46              |
| 40:YU:75:ASN:HB3   | 40:YU:78:THR:H     | 1.81                     | 0.46              |
| 1:QA:411:A:C4      | 1:QA:413:G:H1'     | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:64:G:H4'      | 1:QA:65:U:C5'      | 2.46                     | 0.46              |
| 6:QF:10:LEU:N      | 6:QF:59:TYR:O      | 2.46                     | 0.46              |
| 16:QP:3:LYS:O      | 16:QP:21:VAL:HA    | 2.15                     | 0.46              |
| 17:QQ:74:LEU:HB3   | 17:QQ:75:ARG:H     | 1.63                     | 0.46              |
| 20:QT:33:ILE:HD13  | 20:QT:62:LEU:HB3   | 1.97                     | 0.46              |
| 19:QS:5:LEU:HG     | 50:R4:66:SER:HB3   | 1.98                     | 0.46              |
| 25:RA:2611:U:H5'   | 56:Z7:1:T17:H23    | 1.97                     | 0.46              |
| 25:RA:2676:C:O2    | 25:RA:2732:G:N2    | 2.48                     | 0.46              |
| 25:RA:407:G:H2'    | 25:RA:408:G:H8     | 1.81                     | 0.46              |
| 25:RA:593:G:H1     | 25:RA:664:C:H42    | 1.63                     | 0.46              |
| 30:RG:98:ARG:O     | 30:RG:101:ILE:HG13 | 2.16                     | 0.46              |
| 32:RI:113:ARG:HG3  | 32:RI:131:LYS:HZ2  | 1.80                     | 0.46              |
| 25:RA:2818:G:P     | 37:RR:42:LYS:HZ3   | 2.39                     | 0.46              |
| 38:RS:61:ASN:O     | 38:RS:65:VAL:HG23  | 2.14                     | 0.46              |
| 1:XA:901:A:H8      | 1:XA:901:A:O5'     | 1.98                     | 0.46              |
| 2:XB:163:PHE:CD1   | 2:XB:185:ILE:HG13  | 2.50                     | 0.46              |
| 3:XC:78:GLY:HA3    | 3:XC:83:ARG:HB3    | 1.98                     | 0.46              |
| 9:XI:46:ALA:HA     | 9:XI:78:LYS:HB2    | 1.98                     | 0.46              |
| 10:XJ:62:HIS:H     | 10:XJ:62:HIS:CD2   | 2.33                     | 0.46              |
| 12:XL:45:PRO:HG3   | 12:XL:53:ARG:HD3   | 1.96                     | 0.46              |
| 12:XL:62:SER:O     | 12:XL:64:TYR:N     | 2.48                     | 0.46              |
| 12:XL:7:ILE:HA     | 12:XL:7:ILE:HD13   | 1.82                     | 0.46              |
| 13:XM:36:LYS:HD3   | 13:XM:36:LYS:C     | 2.36                     | 0.46              |
| 6:XF:100:ASN:HB2   | 18:XR:27:GLY:O     | 2.14                     | 0.46              |
| 25:YA:195:A:H5''   | 25:YA:196:A:O5'    | 2.16                     | 0.46              |
| 27:YD:118:VAL:HG22 | 27:YD:119:ALA:N    | 2.31                     | 0.46              |
| 27:YD:35:LYS:HB3   | 27:YD:63:ARG:HA    | 1.98                     | 0.46              |
| 31:YH:152:ARG:HG3  | 31:YH:153:LYS:CD   | 2.35                     | 0.46              |
| 32:YI:3:VAL:O      | 32:YI:18:VAL:HA    | 2.15                     | 0.46              |
| 44:YY:94:LYS:HD2   | 44:YY:101:LYS:HZ3  | 1.81                     | 0.46              |
| 1:QA:1402:C:H2'    | 1:QA:1403:C:O4'    | 2.16                     | 0.46              |
| 1:QA:701:C:H1'     | 1:QA:703:G:N1      | 2.30                     | 0.46              |
| 1:QA:751:U:H2'     | 1:QA:752:G:O4'     | 2.16                     | 0.46              |
| 12:QL:54:LYS:N     | 12:QL:54:LYS:HD2   | 2.30                     | 0.46              |
| 25:RA:1416:G:H2'   | 25:RA:1417:C:C6    | 2.51                     | 0.46              |
| 25:RA:1819:A:H2'   | 27:RD:178:PRO:HB2  | 1.98                     | 0.46              |
| 25:RA:1791:A:N6    | 25:RA:1828:G:O2'   | 2.36                     | 0.46              |
| 25:RA:922:U:H2'    | 25:RA:923:C:C6     | 2.51                     | 0.46              |
| 32:RI:29:TYR:CD2   | 32:RI:30:LEU:HD23  | 2.51                     | 0.46              |
| 38:RS:83:LYS:O     | 38:RS:109:GLY:HA3  | 2.15                     | 0.46              |
| 42:RW:86:LEU:O     | 42:RW:94:ASP:N     | 2.44                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:RY:17:SER:OG    | 44:RY:71:LYS:HD2  | 2.16                     | 0.46              |
| 45:RZ:53:ILE:HG22  | 45:RZ:71:VAL:HG22 | 1.98                     | 0.46              |
| 1:XA:1015:A:H2'    | 1:XA:1016:A:C8    | 2.51                     | 0.46              |
| 1:XA:1158:C:H4'    | 2:XB:133:LYS:NZ   | 2.30                     | 0.46              |
| 1:XA:603:U:H2'     | 1:XA:604:G:H8     | 1.81                     | 0.46              |
| 2:XB:204:ASN:HD22  | 2:XB:205:ASP:N    | 2.13                     | 0.46              |
| 15:XO:56:LEU:O     | 15:XO:60:VAL:HG23 | 2.16                     | 0.46              |
| 23:XW:33:U:O2'     | 23:XW:34:G:H5''   | 2.15                     | 0.46              |
| 47:Y1:96:LYS:H     | 47:Y1:97:LEU:HD12 | 1.81                     | 0.46              |
| 50:Y4:2:LYS:HD2    | 50:Y4:2:LYS:HA    | 1.67                     | 0.46              |
| 25:YA:1154:G:OP2   | 40:YU:58:ARG:NH1  | 2.48                     | 0.46              |
| 25:YA:1203:G:O6    | 25:YA:1204:A:N6   | 2.48                     | 0.46              |
| 25:YA:137(A):G:H2' | 25:YA:139:G:N7    | 2.31                     | 0.46              |
| 25:YA:2882:A:OP1   | 37:YR:96:ARG:NH1  | 2.48                     | 0.46              |
| 27:YD:35:LYS:HE3   | 27:YD:63:ARG:C    | 2.36                     | 0.46              |
| 30:YG:34:LEU:HD12  | 30:YG:100:TRP:CH2 | 2.50                     | 0.46              |
| 36:YQ:136:ALA:O    | 36:YQ:138:ASP:N   | 2.40                     | 0.46              |
| 37:YR:109:ALA:HA   | 37:YR:110:PRO:HD2 | 1.77                     | 0.46              |
| 1:QA:1109:C:OP2    | 3:QC:176:HIS:ND1  | 2.46                     | 0.46              |
| 1:QA:243:A:H4'     | 1:QA:244:U:H3'    | 1.98                     | 0.46              |
| 2:QB:165:VAL:HG23  | 2:QB:166:ASP:H    | 1.81                     | 0.46              |
| 4:QD:75:PHE:HE1    | 4:QD:97:LEU:HD11  | 1.81                     | 0.46              |
| 4:QD:8:VAL:HG13    | 4:QD:21:LEU:HD12  | 1.97                     | 0.46              |
| 1:QA:1330:U:H4'    | 13:QM:23:TYR:CE2  | 2.50                     | 0.46              |
| 1:QA:137:C:O4'     | 16:QP:63:GLY:HA2  | 2.16                     | 0.46              |
| 20:QT:29:LYS:O     | 20:QT:33:ILE:HG12 | 2.16                     | 0.46              |
| 11:QK:54:ARG:NH2   | 23:QW:39:U:O3'    | 2.48                     | 0.46              |
| 52:R6:33:LYS:HG3   | 52:R6:34:LEU:HD13 | 1.98                     | 0.46              |
| 54:R8:39:LYS:O     | 54:R8:43:GLN:HB2  | 2.15                     | 0.46              |
| 25:RA:2696:U:H2'   | 25:RA:2697:G:C8   | 2.50                     | 0.46              |
| 25:RA:811:U:OP2    | 35:RP:29:LYS:N    | 2.42                     | 0.46              |
| 31:RH:87:LEU:HA    | 31:RH:163:TYR:O   | 2.16                     | 0.46              |
| 32:RI:76:THR:OG1   | 32:RI:139:GLN:OE1 | 2.34                     | 0.46              |
| 1:QA:1423:G:OP1    | 34:RO:49:ARG:NH2  | 2.49                     | 0.46              |
| 1:XA:1129:C:H5'    | 1:XA:1130:A:OP1   | 2.16                     | 0.46              |
| 1:XA:1367:C:OP1    | 9:XI:115:GLY:N    | 2.40                     | 0.46              |
| 1:XA:412:A:H4'     | 1:XA:413:G:O5'    | 2.14                     | 0.46              |
| 1:XA:792:A:H4'     | 1:XA:793:U:O5'    | 2.15                     | 0.46              |
| 1:XA:982:U:H5''    | 14:XN:6:LEU:HD21  | 1.97                     | 0.46              |
| 2:XB:114:ARG:O     | 2:XB:118:LEU:HG   | 2.16                     | 0.46              |
| 4:XD:30:LYS:C      | 4:XD:32:ALA:H     | 2.18                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:195:ALA:HB3   | 6:XF:20:ALA:CB     | 2.44                     | 0.46              |
| 6:XF:48:LEU:HG     | 6:XF:57:GLN:HA     | 1.98                     | 0.46              |
| 7:XG:50:ILE:HG21   | 7:XG:61:VAL:HG21   | 1.98                     | 0.46              |
| 18:XR:32:ARG:HA    | 18:XR:69:THR:HG21  | 1.97                     | 0.46              |
| 25:YA:1059:G:H3'   | 25:YA:1060:U:H5''  | 1.97                     | 0.46              |
| 25:YA:2197:U:H1'   | 25:YA:2198:A:C8    | 2.50                     | 0.46              |
| 25:YA:2331:G:H4'   | 46:Y0:43:THR:H     | 1.80                     | 0.46              |
| 25:YA:2790:A:O2'   | 25:YA:2893:G:N3    | 2.48                     | 0.46              |
| 27:YD:121:PRO:CA   | 27:YD:135:PHE:CD2  | 2.81                     | 0.46              |
| 31:YH:167:GLU:HA   | 31:YH:168:PRO:HD3  | 1.79                     | 0.46              |
| 35:YP:135:LEU:HA   | 35:YP:135:LEU:HD23 | 1.74                     | 0.46              |
| 25:YA:661:C:H5''   | 35:YP:15:ARG:NH2   | 2.30                     | 0.46              |
| 56:Z7:3:GLY:HA3    | 56:Z7:4:PRO:HA     | 1.77                     | 0.46              |
| 1:QA:579:G:H5'     | 1:QA:728:A:H1'     | 1.98                     | 0.46              |
| 1:QA:544:G:OP2     | 4:QD:66:ARG:NH2    | 2.49                     | 0.46              |
| 7:QG:150:ALA:O     | 11:QK:57:THR:HG21  | 2.16                     | 0.46              |
| 7:QG:20:ASP:OD1    | 7:QG:21:VAL:N      | 2.48                     | 0.46              |
| 22:QV:6:G:O2'      | 22:QV:49:G:H5'     | 2.16                     | 0.46              |
| 51:R5:56:LYS:CE    | 51:R5:58:LEU:HD23  | 2.46                     | 0.46              |
| 54:R8:50:LEU:C     | 54:R8:53:PRO:HD2   | 2.36                     | 0.46              |
| 55:R9:8:LYS:O      | 55:R9:34:GLN:NE2   | 2.49                     | 0.46              |
| 25:RA:1593:G:H2'   | 25:RA:1594:G:C8    | 2.51                     | 0.46              |
| 25:RA:1773:A:H2'   | 25:RA:1774:C:O4'   | 2.16                     | 0.46              |
| 25:RA:1812:A:H2'   | 25:RA:1813:G:C8    | 2.51                     | 0.46              |
| 25:RA:2154:G:H2'   | 25:RA:2155:G:H8    | 1.79                     | 0.46              |
| 25:RA:2751:G:N7    | 31:RH:2:SER:HB3    | 2.31                     | 0.46              |
| 25:RA:503:A:H4'    | 25:RA:504:U:O5'    | 2.16                     | 0.46              |
| 31:RH:115:VAL:HG11 | 31:RH:148:ILE:HD11 | 1.98                     | 0.46              |
| 31:RH:85:LYS:HA    | 31:RH:85:LYS:HD2   | 1.85                     | 0.46              |
| 32:RI:112:LYS:H    | 32:RI:112:LYS:HG2  | 1.50                     | 0.46              |
| 36:RQ:2:LEU:HD23   | 36:RQ:2:LEU:H      | 1.81                     | 0.46              |
| 45:RZ:23:LYS:HB3   | 45:RZ:38:TYR:CD1   | 2.51                     | 0.46              |
| 1:XA:1213:A:C6     | 1:XA:1215:G:H1'    | 2.51                     | 0.46              |
| 1:XA:1292:U:H2'    | 1:XA:1293:G:C8     | 2.51                     | 0.46              |
| 1:XA:1318:A:H4'    | 19:XS:11:VAL:HG11  | 1.98                     | 0.46              |
| 5:XE:41:VAL:HG13   | 5:XE:113:ALA:HB2   | 1.97                     | 0.46              |
| 9:XI:18:PHE:HD2    | 9:XI:62:TYR:HD2    | 1.62                     | 0.46              |
| 20:XT:26:ASN:O     | 20:XT:30:LYS:HB2   | 2.16                     | 0.46              |
| 47:Y1:80:LEU:HB2   | 47:Y1:81:LYS:H     | 1.61                     | 0.46              |
| 19:XS:4:SER:N      | 50:Y4:67:TYR:HE2   | 2.13                     | 0.46              |
| 35:YP:63:PRO:CA    | 54:Y8:13:ARG:HB3   | 2.46                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1266:G:OP2   | 51:Y5:19:ARG:NH1   | 2.49                     | 0.46              |
| 25:YA:2023:G:H4'   | 25:YA:2617:C:O3'   | 2.16                     | 0.46              |
| 25:YA:2699:C:H2'   | 25:YA:2700:C:O4'   | 2.16                     | 0.46              |
| 25:YA:2836:U:H2'   | 25:YA:2837:G:C8    | 2.51                     | 0.46              |
| 25:YA:578:A:OP1    | 25:YA:1255:U:O2'   | 2.21                     | 0.46              |
| 25:YA:740:U:H2'    | 25:YA:741:G:C8     | 2.51                     | 0.46              |
| 28:YE:116:VAL:O    | 28:YE:117:MET:HB3  | 2.16                     | 0.46              |
| 29:YF:129:PHE:O    | 29:YF:142:TRP:CD1  | 2.69                     | 0.46              |
| 31:YH:15:VAL:CG1   | 31:YH:79:VAL:HG23  | 2.44                     | 0.46              |
| 36:YQ:135:ASP:OD1  | 36:YQ:135:ASP:N    | 2.48                     | 0.46              |
| 42:YW:110:LYS:HG3  | 42:YW:111:HIS:ND1  | 2.31                     | 0.46              |
| 44:YY:84:ARG:HB3   | 44:YY:95:LYS:HD3   | 1.97                     | 0.46              |
| 1:QA:1014:A:H4'    | 19:QS:14:HIS:NE2   | 2.31                     | 0.46              |
| 1:QA:1238:A:OP1    | 1:QA:1335:C:O2'    | 2.22                     | 0.46              |
| 1:QA:1410:G:H2'    | 1:QA:1411:C:C6     | 2.51                     | 0.46              |
| 1:QA:67:C:H2'      | 1:QA:68:G:C8       | 2.51                     | 0.46              |
| 4:QD:15:GLU:HG2    | 4:QD:63:LYS:HG3    | 1.97                     | 0.46              |
| 4:QD:18:LYS:HD3    | 4:QD:20:TYR:CZ     | 2.51                     | 0.46              |
| 13:QM:89:GLY:O     | 13:QM:92:HIS:HB2   | 2.15                     | 0.46              |
| 20:QT:89:ARG:NH2   | 20:QT:105:SER:O    | 2.37                     | 0.46              |
| 23:QY:38:A:H5'     | 25:RA:1913:A:C6    | 2.51                     | 0.46              |
| 47:R1:73:LEU:HB3   | 47:R1:90:ILE:HG23  | 1.97                     | 0.46              |
| 25:RA:1045:A:O2'   | 25:RA:1046:A:OP2   | 2.31                     | 0.46              |
| 25:RA:1047:G:H2'   | 25:RA:1110:G:N1    | 2.31                     | 0.46              |
| 25:RA:2567:G:H2'   | 25:RA:2568:C:C6    | 2.51                     | 0.46              |
| 27:RD:68:LYS:HD2   | 27:RD:70:TRP:CZ2   | 2.51                     | 0.46              |
| 28:RE:63:LEU:HD12  | 28:RE:64:LYS:N     | 2.30                     | 0.46              |
| 31:RH:103:LEU:HD13 | 31:RH:131:VAL:HG11 | 1.97                     | 0.46              |
| 34:RO:31:LYS:HB3   | 34:RO:32:TYR:CD2   | 2.51                     | 0.46              |
| 35:RP:6:LEU:HB3    | 35:RP:7:ARG:H      | 1.55                     | 0.46              |
| 36:RQ:104:PHE:HE2  | 36:RQ:125:LEU:HD11 | 1.80                     | 0.46              |
| 38:RS:24:LEU:HB2   | 38:RS:85:VAL:HG12  | 1.97                     | 0.46              |
| 40:RU:69:CYS:HB3   | 40:RU:106:PHE:HZ   | 1.81                     | 0.46              |
| 41:RV:51:VAL:HG12  | 41:RV:53:GLU:H     | 1.80                     | 0.46              |
| 1:XA:1451:A:H2'    | 1:XA:1451:A:N3     | 2.31                     | 0.46              |
| 12:XL:92:ASP:O     | 12:XL:94:PRO:HD3   | 2.16                     | 0.46              |
| 15:XO:6:GLU:CD     | 15:XO:6:GLU:H      | 2.15                     | 0.46              |
| 18:XR:73:ALA:HB3   | 18:XR:79:LEU:HD12  | 1.98                     | 0.46              |
| 22:XV:2:C:H2'      | 22:XV:3:G:H5'      | 1.98                     | 0.46              |
| 25:YA:2599:G:OP2   | 27:YD:236:GLY:HA2  | 2.15                     | 0.46              |
| 25:YA:755:C:H2'    | 25:YA:756:C:C6     | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:YB:111:U:H2'    | 26:YB:112:G:H8     | 1.80                     | 0.46              |
| 28:YE:70:ALA:O     | 28:YE:72:VAL:N     | 2.49                     | 0.46              |
| 31:YH:103:LEU:HD23 | 31:YH:115:VAL:HB   | 1.97                     | 0.46              |
| 35:YP:138:LEU:C    | 35:YP:140:ALA:H    | 2.18                     | 0.46              |
| 41:YV:19:LYS:HA    | 41:YV:94:LEU:O     | 2.15                     | 0.46              |
| 1:QA:1001:G:H2'    | 1:QA:1002:G:O4'    | 2.16                     | 0.45              |
| 1:QA:1012:U:H2'    | 1:QA:1013:G:C8     | 2.51                     | 0.45              |
| 1:QA:1349:A:P      | 9:QI:118:LYS:HZ3   | 2.39                     | 0.45              |
| 4:QD:121:VAL:O     | 4:QD:134:ASP:HA    | 2.16                     | 0.45              |
| 4:QD:53:ASP:O      | 4:QD:57:ARG:HD2    | 2.16                     | 0.45              |
| 8:QH:20:TYR:HA     | 8:QH:65:TYR:CZ     | 2.51                     | 0.45              |
| 13:QM:84:ILE:HD12  | 13:QM:84:ILE:HA    | 1.75                     | 0.45              |
| 52:R6:44:ARG:O     | 52:R6:45:LYS:HB2   | 2.16                     | 0.45              |
| 25:RA:1203:G:H3'   | 25:RA:1204:A:H5''  | 1.98                     | 0.45              |
| 25:RA:1336:A:H2'   | 25:RA:1337:G:C8    | 2.51                     | 0.45              |
| 25:RA:2019:A:H4'   | 40:RU:34:LYS:HD2   | 1.99                     | 0.45              |
| 25:RA:2645:G:H3'   | 25:RA:2646:C:H5'   | 1.97                     | 0.45              |
| 26:RB:15:A:H1'     | 26:RB:109:G:N9     | 2.31                     | 0.45              |
| 31:RH:120:GLY:HA3  | 31:RH:140:LYS:NZ   | 2.31                     | 0.45              |
| 35:RP:101:VAL:HG23 | 35:RP:107:LYS:H    | 1.81                     | 0.45              |
| 36:RQ:29:PHE:N     | 36:RQ:105:GLU:OE2  | 2.40                     | 0.45              |
| 37:RR:37:THR:OG1   | 37:RR:40:LYS:HG3   | 2.17                     | 0.45              |
| 1:XA:599:C:H42     | 1:XA:639:G:H1      | 1.64                     | 0.45              |
| 2:XB:70:PHE:O      | 2:XB:93:VAL:N      | 2.34                     | 0.45              |
| 1:XA:8:A:N6        | 4:XD:205:GLU:O     | 2.48                     | 0.45              |
| 1:XA:1117:G:H5''   | 9:XI:104:ARG:NH1   | 2.31                     | 0.45              |
| 13:XM:58:GLU:O     | 13:XM:62:ASN:ND2   | 2.33                     | 0.45              |
| 52:Y6:33:LYS:HB2   | 52:Y6:33:LYS:HE2   | 1.76                     | 0.45              |
| 25:YA:229:A:OP1    | 25:YA:229:A:H4'    | 2.16                     | 0.45              |
| 25:YA:2867:G:O2'   | 25:YA:2868:A:C8    | 2.69                     | 0.45              |
| 25:YA:755:C:H2'    | 25:YA:756:C:H6     | 1.81                     | 0.45              |
| 27:YD:10:THR:OG1   | 27:YD:13:ARG:HB2   | 2.16                     | 0.45              |
| 28:YE:108:SER:HB3  | 28:YE:165:VAL:HG21 | 1.99                     | 0.45              |
| 29:YF:129:PHE:C    | 29:YF:131:GLY:H    | 2.18                     | 0.45              |
| 31:YH:106:THR:HG22 | 31:YH:112:PRO:HB3  | 1.97                     | 0.45              |
| 35:YP:58:THR:O     | 35:YP:61:ARG:CZ    | 2.65                     | 0.45              |
| 44:YY:51:VAL:HG13  | 44:YY:52:SER:N     | 2.28                     | 0.45              |
| 1:QA:1342:C:H2'    | 1:QA:1343:G:C8     | 2.51                     | 0.45              |
| 1:QA:407:G:OP1     | 4:QD:3:ARG:NH1     | 2.49                     | 0.45              |
| 1:QA:743:U:H2'     | 1:QA:744:C:C6      | 2.50                     | 0.45              |
| 3:QC:19:GLU:HA     | 3:QC:54:ARG:HH12   | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:QI:126:SER:O     | 9:QI:128:ARG:N     | 2.45                     | 0.45              |
| 9:QI:45:ALA:O      | 9:QI:48:GLU:HG2    | 2.15                     | 0.45              |
| 19:QS:32:LYS:HA    | 19:QS:50:ALA:HB3   | 1.98                     | 0.45              |
| 25:RA:1228:G:OP1   | 40:RU:13:LYS:HG2   | 2.15                     | 0.45              |
| 25:RA:622:G:H2'    | 25:RA:623:G:H8     | 1.81                     | 0.45              |
| 35:RP:77:ARG:HB2   | 35:RP:78:PRO:HD2   | 1.98                     | 0.45              |
| 39:RT:26:ASP:HB2   | 39:RT:90:GLN:O     | 2.16                     | 0.45              |
| 1:XA:1346:A:H1'    | 1:XA:1348:U:C6     | 2.52                     | 0.45              |
| 1:XA:686:U:O2'     | 11:XK:42:TRP:NE1   | 2.47                     | 0.45              |
| 2:XB:55:PHE:HD1    | 2:XB:58:ILE:HG13   | 1.81                     | 0.45              |
| 19:XS:47:HIS:O     | 19:XS:62:ILE:HG12  | 2.17                     | 0.45              |
| 47:Y1:58:ILE:N     | 47:Y1:58:ILE:HD12  | 2.30                     | 0.45              |
| 47:Y1:91:LYS:HE3   | 47:Y1:91:LYS:HA    | 1.98                     | 0.45              |
| 48:Y2:4:SER:OG     | 48:Y2:5:GLU:OE1    | 2.23                     | 0.45              |
| 30:YG:6:ALA:N      | 50:Y4:23:GLU:HG2   | 2.28                     | 0.45              |
| 25:YA:2788:C:O2'   | 25:YA:2809:A:N3    | 2.40                     | 0.45              |
| 27:YD:137:PRO:O    | 27:YD:140:THR:HG23 | 2.16                     | 0.45              |
| 29:YF:11:VAL:HA    | 29:YF:125:LEU:O    | 2.16                     | 0.45              |
| 37:YR:24:GLN:HE21  | 37:YR:44:LEU:HG    | 1.81                     | 0.45              |
| 37:YR:78:LYS:O     | 37:YR:83:ILE:HG12  | 2.16                     | 0.45              |
| 38:YS:58:LEU:N     | 38:YS:58:LEU:CD2   | 2.73                     | 0.45              |
| 1:QA:1129:C:H4'    | 1:QA:1130:A:H5'    | 1.98                     | 0.45              |
| 12:QL:113:ARG:HH21 | 12:QL:116:SER:HB2  | 1.81                     | 0.45              |
| 6:QF:99:ALA:HB1    | 18:QR:23:LYS:NZ    | 2.31                     | 0.45              |
| 25:RA:1469:A:H2'   | 25:RA:1470:G:O4'   | 2.16                     | 0.45              |
| 25:RA:2116:G:N1    | 25:RA:2162:G:OP1   | 2.50                     | 0.45              |
| 25:RA:2543:G:H2'   | 25:RA:2544:G:C8    | 2.51                     | 0.45              |
| 27:RD:121:PRO:HB3  | 27:RD:135:PHE:CE2  | 2.52                     | 0.45              |
| 25:RA:468:G:H5'    | 29:RF:60:SER:HB2   | 1.98                     | 0.45              |
| 37:RR:33:ARG:HG2   | 37:RR:34:ILE:N     | 2.30                     | 0.45              |
| 1:XA:1036:G:H5'    | 1:XA:1037:C:OP2    | 2.16                     | 0.45              |
| 1:XA:222:U:H2'     | 1:XA:223:U:C6      | 2.52                     | 0.45              |
| 1:XA:411:A:C4      | 1:XA:413:G:H1'     | 2.51                     | 0.45              |
| 1:XA:736:C:H2'     | 1:XA:737:A:C8      | 2.52                     | 0.45              |
| 1:XA:69:G:H2'      | 1:XA:73:G:C8       | 2.51                     | 0.45              |
| 2:XB:217:ARG:HB2   | 2:XB:217:ARG:HE    | 1.54                     | 0.45              |
| 3:XC:48:TYR:OH     | 3:XC:122:GLU:OE2   | 2.22                     | 0.45              |
| 8:XH:86:ILE:HG13   | 8:XH:133:LEU:HD22  | 1.98                     | 0.45              |
| 9:XI:114:TYR:N     | 9:XI:114:TYR:HD1   | 2.14                     | 0.45              |
| 12:XL:44:THR:HA    | 12:XL:45:PRO:HD3   | 1.68                     | 0.45              |
| 25:YA:83:G:N2      | 25:YA:103:A:OP2    | 2.45                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2159:G:H2'   | 25:YA:2160:G:H8   | 1.81                     | 0.45              |
| 25:YA:2712:U:HO2'  | 25:YA:2712(A):A:P | 2.38                     | 0.45              |
| 25:YA:2817:G:OP1   | 37:YR:99:LYS:NZ   | 2.44                     | 0.45              |
| 25:YA:844:C:H2'    | 25:YA:845:G:O4'   | 2.16                     | 0.45              |
| 31:YH:109:PHE:CE1  | 31:YH:152:ARG:HD3 | 2.51                     | 0.45              |
| 31:YH:86:GLU:O     | 31:YH:87:LEU:HB2  | 2.16                     | 0.45              |
| 32:YI:131:LYS:HB3  | 32:YI:132:PRO:HA  | 1.98                     | 0.45              |
| 32:YI:51:ILE:O     | 32:YI:55:ALA:N    | 2.31                     | 0.45              |
| 35:YP:27:HIS:N     | 35:YP:27:HIS:ND1  | 2.64                     | 0.45              |
| 37:YR:51:LEU:HD12  | 37:YR:70:LEU:HG   | 1.97                     | 0.45              |
| 40:YU:66:ASN:O     | 40:YU:70:ARG:HB2  | 2.17                     | 0.45              |
| 40:YU:68:ALA:O     | 40:YU:71:GLN:HB2  | 2.16                     | 0.45              |
| 25:YA:336:C:HO2'   | 44:YY:35:TYR:HH   | 1.65                     | 0.45              |
| 44:YY:87:LYS:HA    | 44:YY:92:ASN:HB3  | 1.98                     | 0.45              |
| 4:QD:103:ASN:OD1   | 4:QD:114:ARG:NE   | 2.49                     | 0.45              |
| 1:QA:1375:A:H4'    | 7:QG:29:LYS:HE3   | 1.97                     | 0.45              |
| 3:QC:23:TYR:CD1    | 10:QJ:10:GLY:HA2  | 2.51                     | 0.45              |
| 14:QN:32:SER:O     | 14:QN:32:SER:OG   | 2.26                     | 0.45              |
| 19:QS:67:VAL:HG21  | 50:R4:60:GLN:OE1  | 2.16                     | 0.45              |
| 20:QT:26:ASN:HB2   | 20:QT:71:THR:HG23 | 1.97                     | 0.45              |
| 25:RA:1210:A:H4'   | 25:RA:1211:U:O5'  | 2.16                     | 0.45              |
| 25:RA:1220:A:H5'   | 25:RA:1221:C:OP2  | 2.16                     | 0.45              |
| 25:RA:1527:G:H2'   | 25:RA:1543:A:N1   | 2.30                     | 0.45              |
| 25:RA:2307:G:H1'   | 25:RA:2308:G:C2   | 2.52                     | 0.45              |
| 25:RA:2695:C:H2'   | 25:RA:2696:U:C6   | 2.52                     | 0.45              |
| 25:RA:898:C:C2'    | 25:RA:899:A:H5'   | 2.47                     | 0.45              |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:H   | 1.82                     | 0.45              |
| 27:RD:30:GLU:HG3   | 27:RD:63:ARG:CZ   | 2.47                     | 0.45              |
| 31:RH:170:ARG:HB3  | 31:RH:171:LEU:H   | 1.52                     | 0.45              |
| 38:RS:16:ASN:HA    | 38:RS:19:LYS:HD3  | 1.99                     | 0.45              |
| 37:RR:103:ARG:NH1  | 42:RW:40:ASN:OD1  | 2.50                     | 0.45              |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:C8 | 2.51                     | 0.45              |
| 1:XA:1316:G:N1     | 1:XA:1319:A:OP2   | 2.48                     | 0.45              |
| 1:XA:337:C:H2'     | 1:XA:338:A:H8     | 1.80                     | 0.45              |
| 1:XA:620:C:H2'     | 1:XA:621:A:O4'    | 2.17                     | 0.45              |
| 2:XB:140:HIS:HA    | 2:XB:143:GLU:OE1  | 2.17                     | 0.45              |
| 7:XG:45:ASP:O      | 7:XG:49:ILE:HG12  | 2.17                     | 0.45              |
| 19:XS:63:THR:HG23  | 19:XS:66:MET:HG2  | 1.99                     | 0.45              |
| 25:YA:1454:U:H5'   | 37:YR:63:ARG:NE   | 2.32                     | 0.45              |
| 25:YA:1678:G:N2    | 25:YA:1989:G:H22  | 2.14                     | 0.45              |
| 25:YA:2591:C:H2'   | 25:YA:2592:G:C8   | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:2847:U:P    | 39:YT:98:LYS:HZ3  | 2.39                     | 0.45              |
| 35:YP:124:LYS:HA  | 35:YP:143:GLY:O   | 2.16                     | 0.45              |
| 40:YU:58:ARG:HA   | 40:YU:61:TRP:CE3  | 2.52                     | 0.45              |
| 1:QA:1172:C:H2'   | 1:QA:1173:G:H8    | 1.79                     | 0.45              |
| 1:QA:1227:A:OP2   | 13:QM:111:LYS:HE3 | 2.16                     | 0.45              |
| 1:QA:1298:C:H4'   | 1:QA:1299:A:C4    | 2.51                     | 0.45              |
| 1:QA:1435:G:H2'   | 1:QA:1436:U:C6    | 2.51                     | 0.45              |
| 1:QA:266:G:O2'    | 1:QA:268:C:OP2    | 2.35                     | 0.45              |
| 1:QA:939:G:H5''   | 7:QG:102:ARG:NH2  | 2.32                     | 0.45              |
| 8:QH:104:ARG:O    | 8:QH:107:LEU:HB2  | 2.16                     | 0.45              |
| 10:QJ:51:ARG:NH2  | 14:QN:58:LYS:HZ1  | 2.15                     | 0.45              |
| 23:QW:76:A:N6     | 25:RA:2422:A:O4'  | 2.49                     | 0.45              |
| 52:R6:26:ASN:ND2  | 52:R6:35:GLU:OE2  | 2.49                     | 0.45              |
| 25:RA:1101:U:H2'  | 25:RA:1102:C:C6   | 2.52                     | 0.45              |
| 25:RA:1860:G:H2'  | 25:RA:1861:G:C8   | 2.52                     | 0.45              |
| 25:RA:2245:U:C5'  | 25:RA:2246:G:H5'  | 2.46                     | 0.45              |
| 25:RA:2291:U:H2'  | 25:RA:2292:C:C6   | 2.52                     | 0.45              |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:H8   | 1.81                     | 0.45              |
| 1:QA:1443:G:N2    | 25:RA:2864:G:OP1  | 2.43                     | 0.45              |
| 25:RA:443:A:H3'   | 29:RF:45:ARG:HH12 | 1.82                     | 0.45              |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA2 | 1.97                     | 0.45              |
| 34:RO:48:PRO:O    | 34:RO:49:ARG:HG2  | 2.17                     | 0.45              |
| 35:RP:88:LEU:HD12 | 35:RP:95:VAL:HG11 | 1.99                     | 0.45              |
| 45:RZ:118:GLN:O   | 45:RZ:120:ILE:N   | 2.46                     | 0.45              |
| 1:XA:1118:C:P     | 9:XI:104:ARG:HH11 | 2.39                     | 0.45              |
| 1:XA:1285:A:H4'   | 1:XA:1286:A:O5'   | 2.16                     | 0.45              |
| 1:XA:255:G:C6     | 1:XA:256:U:O4     | 2.69                     | 0.45              |
| 1:XA:64:G:H5''    | 1:XA:65:U:OP1     | 2.16                     | 0.45              |
| 7:XG:15:ASP:OD1   | 7:XG:44:TYR:OH    | 2.35                     | 0.45              |
| 48:Y2:24:LEU:HD23 | 48:Y2:24:LEU:HA   | 1.67                     | 0.45              |
| 25:YA:1020:A:N1   | 25:YA:1141:U:H2'  | 2.32                     | 0.45              |
| 25:YA:1113:U:H2'  | 25:YA:1114:G:H8   | 1.81                     | 0.45              |
| 25:YA:1533:C:H2'  | 25:YA:1534:G:N7   | 2.31                     | 0.45              |
| 25:YA:807:U:O2'   | 25:YA:2060:A:N1   | 2.46                     | 0.45              |
| 25:YA:2086:U:H2'  | 25:YA:2087:G:C8   | 2.51                     | 0.45              |
| 25:YA:2537:U:H2'  | 25:YA:2538:C:C6   | 2.51                     | 0.45              |
| 25:YA:306:U:H2'   | 25:YA:307:G:O4'   | 2.17                     | 0.45              |
| 41:YV:36:PRO:HA   | 41:YV:56:SER:OG   | 2.16                     | 0.45              |
| 44:YY:56:PRO:O    | 44:YY:58:GLY:N    | 2.49                     | 0.45              |
| 1:QA:946:A:N6     | 1:QA:1234:C:H42   | 2.14                     | 0.45              |
| 1:QA:1252:A:H61   | 1:QA:1285:A:H61   | 1.64                     | 0.45              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:QA:129(A):G:N2    | 1:QA:188:U:O2'    | 2.50                     | 0.45              |
| 1:QA:518:C:H2'      | 1:QA:530:G:N3     | 2.32                     | 0.45              |
| 1:QA:565:U:H5''     | 1:QA:566:G:H2'    | 1.98                     | 0.45              |
| 6:QF:45:LEU:HD12    | 6:QF:59:TYR:HD2   | 1.82                     | 0.45              |
| 20:QT:64:ASP:CG     | 20:QT:81:LYS:HZ2  | 2.20                     | 0.45              |
| 25:RA:1220:A:OP2    | 40:RU:19:LYS:NZ   | 2.35                     | 0.45              |
| 25:RA:1637:A:H4'    | 25:RA:2711:A:O2'  | 2.17                     | 0.45              |
| 25:RA:195:A:H5''    | 25:RA:196:A:O5'   | 2.16                     | 0.45              |
| 25:RA:2692:C:H2'    | 25:RA:2693:A:H8   | 1.82                     | 0.45              |
| 25:RA:627:A:H4'     | 25:RA:628:G:H5'   | 1.99                     | 0.45              |
| 25:RA:774:A:H2      | 25:RA:787:U:O2'   | 2.00                     | 0.45              |
| 30:RG:106:LEU:HA    | 30:RG:110:ALA:HB3 | 1.98                     | 0.45              |
| 33:RN:19:GLU:HB2    | 33:RN:56:ASN:HD22 | 1.80                     | 0.45              |
| 35:RP:18:ARG:HD2    | 35:RP:27:HIS:HD2  | 1.81                     | 0.45              |
| 28:RE:111:ARG:HA    | 37:RR:1:MET:SD    | 2.57                     | 0.45              |
| 37:RR:42:LYS:HA     | 37:RR:45:ARG:HD2  | 1.98                     | 0.45              |
| 38:RS:10:ARG:O      | 38:RS:14:VAL:HG12 | 2.17                     | 0.45              |
| 1:XA:1152:A:H5''    | 10:XJ:13:HIS:CD2  | 2.52                     | 0.45              |
| 1:XA:1321:C:C3'     | 1:XA:1322:C:H5''  | 2.45                     | 0.45              |
| 1:XA:1513:A:H2'     | 1:XA:1514:C:C6    | 2.52                     | 0.45              |
| 1:XA:276:G:OP1      | 17:XQ:12:SER:OG   | 2.23                     | 0.45              |
| 1:XA:485:G:O2'      | 1:XA:486:U:O5'    | 2.34                     | 0.45              |
| 3:XC:153:VAL:HG22   | 3:XC:198:VAL:HG22 | 1.98                     | 0.45              |
| 5:XE:99:GLY:N       | 5:XE:117:ASP:OD1  | 2.47                     | 0.45              |
| 8:XH:75:ARG:HA      | 8:XH:76:PRO:HD2   | 1.71                     | 0.45              |
| 15:XO:32:LEU:HD11   | 15:XO:62:GLN:HG2  | 1.99                     | 0.45              |
| 17:XQ:43:LEU:HD12   | 17:XQ:68:ARG:HG2  | 1.97                     | 0.45              |
| 19:XS:68:GLY:H      | 50:Y4:59:PHE:HZ   | 1.60                     | 0.45              |
| 46:Y0:23:VAL:HA     | 46:Y0:38:VAL:HA   | 1.99                     | 0.45              |
| 52:Y6:15:GLU:CD     | 52:Y6:41:PRO:HB3  | 2.37                     | 0.45              |
| 25:YA:1045:A:N3     | 25:YA:1047:G:N2   | 2.65                     | 0.45              |
| 25:YA:1061:U:H5'    | 25:YA:1070:A:O2'  | 2.16                     | 0.45              |
| 25:YA:1069:A:H2'    | 25:YA:1073:A:N7   | 2.31                     | 0.45              |
| 25:YA:2022:U:O2'    | 25:YA:2616:C:O2'  | 2.22                     | 0.45              |
| 25:YA:2693:A:H2'    | 25:YA:2694:G:C8   | 2.51                     | 0.45              |
| 25:YA:651:G:H4'     | 54:Y8:18:ALA:HB3  | 1.99                     | 0.45              |
| 25:YA:848:G:H2'     | 25:YA:849:A:C8    | 2.52                     | 0.45              |
| 25:YA:1142(A):A:H4' | 33:YN:25:ARG:HH22 | 1.80                     | 0.45              |
| 39:YT:6:LEU:HA      | 39:YT:9:LEU:HB2   | 1.99                     | 0.45              |
| 41:YV:19:LYS:HG3    | 41:YV:95:LEU:HD23 | 1.98                     | 0.45              |
| 44:YY:101:LYS:HG2   | 44:YY:102:CYS:H   | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:481:G:O2'     | 1:QA:482:A:O5'     | 2.35                     | 0.45              |
| 2:QB:76:GLN:O      | 2:QB:208:ILE:HG12  | 2.17                     | 0.45              |
| 11:QK:41:THR:HG21  | 11:QK:71:LYS:HB2   | 1.99                     | 0.45              |
| 12:QL:109:GLY:HA3  | 12:QL:121:GLY:O    | 2.17                     | 0.45              |
| 13:QM:3:ARG:HB3    | 50:R4:34:GLU:HB3   | 1.98                     | 0.45              |
| 50:R4:10:VAL:HA    | 50:R4:11:PRO:HD2   | 1.75                     | 0.45              |
| 25:RA:1012:U:O4    | 33:RN:25:ARG:HA    | 2.16                     | 0.45              |
| 25:RA:2022:U:O2'   | 25:RA:2617:C:H5'   | 2.16                     | 0.45              |
| 25:RA:307:G:N2     | 25:RA:330:A:H62    | 2.14                     | 0.45              |
| 25:RA:479:A:N3     | 25:RA:481:G:H5''   | 2.32                     | 0.45              |
| 26:RB:89(A):A:H8   | 26:RB:89(A):A:O5'  | 2.00                     | 0.45              |
| 27:RD:76:PRO:HB2   | 27:RD:116:GLN:OE1  | 2.17                     | 0.45              |
| 30:RG:10:LYS:O     | 30:RG:14:GLU:HB3   | 2.17                     | 0.45              |
| 32:RI:101:LEU:HD22 | 32:RI:107:VAL:HB   | 1.98                     | 0.45              |
| 36:RQ:111:GLU:C    | 36:RQ:113:GLN:H    | 2.19                     | 0.45              |
| 37:RR:78:LYS:HE2   | 37:RR:83:ILE:HD11  | 1.98                     | 0.45              |
| 44:RY:68:HIS:CE1   | 44:RY:70:SER:HB3   | 2.52                     | 0.45              |
| 44:RY:90:LEU:HB2   | 44:RY:91:GLU:H     | 1.63                     | 0.45              |
| 1:XA:1223:C:P      | 19:XS:78:ARG:HH12  | 2.39                     | 0.45              |
| 1:XA:1446:A:HO2'   | 1:XA:1447:G:P      | 2.39                     | 0.45              |
| 1:XA:217:C:O2'     | 1:XA:466:C:N4      | 2.49                     | 0.45              |
| 1:XA:863:U:O2'     | 1:XA:865:A:N7      | 2.45                     | 0.45              |
| 48:Y2:21:LEU:O     | 48:Y2:25:VAL:HG23  | 2.17                     | 0.45              |
| 25:YA:122:G:OP1    | 25:YA:149:A:O2'    | 2.27                     | 0.45              |
| 25:YA:2123:G:H1    | 25:YA:2175:C:N4    | 2.11                     | 0.45              |
| 1:XA:1443:G:N2     | 25:YA:2864:G:OP1   | 2.37                     | 0.45              |
| 25:YA:407:G:H2'    | 25:YA:408:G:C8     | 2.52                     | 0.45              |
| 27:YD:44:ASN:ND2   | 27:YD:44:ASN:N     | 2.64                     | 0.45              |
| 30:YG:146:TYR:O    | 30:YG:149:VAL:HG22 | 2.16                     | 0.45              |
| 1:XA:1446:A:C6     | 39:YT:118:ARG:HD2  | 2.52                     | 0.45              |
| 1:QA:1016:A:H2'    | 1:QA:1017:G:O4'    | 2.17                     | 0.45              |
| 1:QA:1504:G:OP1    | 1:QA:1507:A:H4'    | 2.17                     | 0.45              |
| 1:QA:244:U:H4'     | 1:QA:245:C:O5'     | 2.16                     | 0.45              |
| 1:QA:696:A:H2'     | 1:QA:697:U:C6      | 2.52                     | 0.45              |
| 7:QG:113:GLU:CG    | 7:QG:119:ARG:HG2   | 2.47                     | 0.45              |
| 7:QG:49:ILE:O      | 7:QG:53:LYS:HB3    | 2.16                     | 0.45              |
| 48:R2:41:ILE:HD11  | 48:R2:44:LEU:HB2   | 1.98                     | 0.45              |
| 25:RA:1029:A:OP1   | 36:RQ:128:LYS:HE3  | 2.17                     | 0.45              |
| 25:RA:1827:C:OP2   | 27:RD:222:ARG:NH1  | 2.44                     | 0.45              |
| 25:RA:2308:G:C6    | 25:RA:2311:A:N1    | 2.85                     | 0.45              |
| 25:RA:345:A:H5''   | 25:RA:346:A:OP1    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:463:G:N2     | 25:RA:466:A:OP2   | 2.48                     | 0.45              |
| 25:RA:57:C:H2'     | 25:RA:58:G:O4'    | 2.17                     | 0.45              |
| 28:RE:46:ALA:HB2   | 28:RE:82:ARG:HA   | 1.98                     | 0.45              |
| 31:RH:125:VAL:HG13 | 31:RH:126:PRO:HB3 | 1.99                     | 0.45              |
| 25:RA:805:G:OP2    | 35:RP:41:ARG:HG2  | 2.17                     | 0.45              |
| 45:RZ:53:ILE:H     | 45:RZ:71:VAL:CG1  | 2.30                     | 0.45              |
| 1:XA:1192:C:O2     | 5:XE:25:ARG:NH2   | 2.34                     | 0.45              |
| 2:XB:115:LEU:HD13  | 2:XB:145:LEU:HB3  | 1.98                     | 0.45              |
| 4:XD:86:LYS:H      | 4:XD:86:LYS:HD2   | 1.82                     | 0.45              |
| 13:XM:65:LYS:O     | 13:XM:70:LEU:HD23 | 2.17                     | 0.45              |
| 16:XP:17:TYR:CE2   | 16:XP:41:PRO:HG3  | 2.52                     | 0.45              |
| 23:XW:19:G:H22     | 23:XW:56:C:H42    | 1.65                     | 0.45              |
| 47:Y1:79:GLY:N     | 47:Y1:80:LEU:HD23 | 2.32                     | 0.45              |
| 49:Y3:31:LEU:O     | 49:Y3:32:GLN:HB2  | 2.17                     | 0.45              |
| 50:Y4:22:ILE:HG22  | 50:Y4:23:GLU:H    | 1.82                     | 0.45              |
| 50:Y4:16:CYS:HB3   | 50:Y4:33:VAL:HB   | 1.98                     | 0.45              |
| 25:YA:1028:A:N6    | 25:YA:1125:G:H2'  | 2.32                     | 0.45              |
| 25:YA:27:G:H22     | 25:YA:512:G:H2'   | 1.80                     | 0.45              |
| 25:YA:286:C:H2'    | 25:YA:287:C:C6    | 2.52                     | 0.45              |
| 25:YA:874:G:H2'    | 25:YA:875:G:H8    | 1.81                     | 0.45              |
| 26:YB:12:C:O2      | 46:Y0:74:ARG:HD2  | 2.17                     | 0.45              |
| 28:YE:67:PHE:O     | 28:YE:69:LYS:N    | 2.49                     | 0.45              |
| 25:YA:2636:U:OP2   | 28:YE:79:ARG:NH1  | 2.49                     | 0.45              |
| 31:YH:85:LYS:HA    | 31:YH:85:LYS:HD2  | 1.89                     | 0.45              |
| 39:YT:102:ILE:HA   | 39:YT:105:LEU:CD2 | 2.47                     | 0.45              |
| 1:QA:64:G:H4'      | 1:QA:65:U:O5'     | 2.16                     | 0.45              |
| 7:QG:45:ASP:O      | 7:QG:49:ILE:HG12  | 2.16                     | 0.45              |
| 8:QH:92:ARG:HD3    | 8:QH:92:ARG:HA    | 1.77                     | 0.45              |
| 1:QA:1060:C:O2'    | 10:QJ:56:HIS:ND1  | 2.46                     | 0.45              |
| 11:QK:91:ARG:NH1   | 11:QK:110:ASP:OD2 | 2.47                     | 0.45              |
| 12:QL:71:PRO:HG3   | 12:QL:99:HIS:HD2  | 1.82                     | 0.45              |
| 51:R5:58:LEU:CD1   | 51:R5:58:LEU:N    | 2.73                     | 0.45              |
| 52:R6:34:LEU:HD13  | 52:R6:34:LEU:H    | 1.82                     | 0.45              |
| 25:RA:856:C:HO2'   | 25:RA:857:C:P     | 2.39                     | 0.45              |
| 29:RF:45:ARG:CG    | 29:RF:45:ARG:HH11 | 2.29                     | 0.45              |
| 34:RO:22:ILE:HG12  | 34:RO:41:ALA:HA   | 1.98                     | 0.45              |
| 45:RZ:181:GLU:HB3  | 45:RZ:182:LYS:HD3 | 1.98                     | 0.45              |
| 1:XA:304:U:H2'     | 1:XA:305:G:C8     | 2.52                     | 0.45              |
| 13:XM:115:LYS:HE3  | 13:XM:115:LYS:HB2 | 1.75                     | 0.45              |
| 19:XS:66:MET:HB2   | 19:XS:74:PHE:CZ   | 2.52                     | 0.45              |
| 20:XT:87:LYS:HD2   | 20:XT:87:LYS:HA   | 1.74                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1021:A:H61   | 25:YA:1142(A):A:N6 | 2.01                     | 0.45              |
| 25:YA:1231:G:H2'   | 25:YA:1232:G:H8    | 1.82                     | 0.45              |
| 25:YA:1534:G:N3    | 25:YA:1534:G:H2'   | 2.32                     | 0.45              |
| 25:YA:1380:G:O2'   | 25:YA:1569:A:N6    | 2.50                     | 0.45              |
| 25:YA:548:A:H8     | 25:YA:548:A:O5'    | 2.00                     | 0.45              |
| 25:YA:1500:G:O2'   | 27:YD:100:GLY:O    | 2.24                     | 0.45              |
| 31:YH:45:VAL:HG13  | 31:YH:45:VAL:O     | 2.17                     | 0.45              |
| 32:YI:120:ILE:HD11 | 32:YI:126:TYR:CZ   | 2.52                     | 0.45              |
| 32:YI:88:ILE:HG12  | 32:YI:122:GLU:N    | 2.31                     | 0.45              |
| 43:YX:60:ARG:HH22  | 53:Y7:47:ARG:NH1   | 2.14                     | 0.45              |
| 1:QA:1176:A:H2'    | 1:QA:1177:G:H5'    | 1.98                     | 0.45              |
| 1:QA:299:G:H2'     | 1:QA:300:A:C8      | 2.52                     | 0.45              |
| 1:QA:429:U:H1'     | 1:QA:430:A:H5''    | 1.98                     | 0.45              |
| 1:QA:880:C:OP2     | 12:QL:9:GLN:HG3    | 2.17                     | 0.45              |
| 1:QA:892:A:O2'     | 1:QA:1415:G:H4'    | 2.17                     | 0.45              |
| 8:QH:6:ILE:O       | 8:QH:10:LEU:HG     | 2.17                     | 0.45              |
| 8:QH:6:ILE:HB      | 8:QH:85:ARG:HH11   | 1.82                     | 0.45              |
| 1:QA:1348:U:H4'    | 9:QI:120:ARG:HD2   | 1.98                     | 0.45              |
| 12:QL:11:VAL:HG13  | 17:QQ:29:HIS:HD2   | 1.82                     | 0.45              |
| 13:QM:92:HIS:CD2   | 13:QM:110:ARG:HH21 | 2.35                     | 0.45              |
| 51:R5:36:CYS:SG    | 51:R5:48:GLU:HB3   | 2.57                     | 0.45              |
| 35:RP:64:LYS:HB2   | 54:R8:25:MET:HG3   | 1.98                     | 0.45              |
| 25:RA:270:A:OP2    | 25:RA:270(Y):G:N1  | 2.38                     | 0.45              |
| 26:RB:31:C:N4      | 26:RB:51:G:H1      | 2.15                     | 0.45              |
| 27:RD:85:ASP:HA    | 27:RD:86:PRO:HD2   | 1.72                     | 0.45              |
| 28:RE:107:THR:O    | 28:RE:190:GLY:HA2  | 2.17                     | 0.45              |
| 29:RF:161:GLU:OE2  | 29:RF:164:ARG:NH1  | 2.50                     | 0.45              |
| 30:RG:102:PHE:O    | 30:RG:106:LEU:N    | 2.50                     | 0.45              |
| 25:RA:2311:A:C8    | 30:RG:88:ILE:HD11  | 2.52                     | 0.45              |
| 31:RH:52:VAL:HG21  | 31:RH:69:ARG:HA    | 1.98                     | 0.45              |
| 32:RI:14:ASP:N     | 32:RI:14:ASP:OD1   | 2.50                     | 0.45              |
| 1:XA:1318:A:H4'    | 19:XS:11:VAL:CG1   | 2.47                     | 0.45              |
| 9:XI:111:ARG:HH22  | 10:XJ:62:HIS:CE1   | 2.35                     | 0.45              |
| 19:XS:24:ALA:O     | 19:XS:25:LYS:HB3   | 2.17                     | 0.45              |
| 20:XT:33:ILE:HG23  | 20:XT:63:ILE:HG12  | 1.99                     | 0.45              |
| 25:YA:2395:C:O2'   | 47:Y1:30:VAL:HG12  | 2.17                     | 0.45              |
| 25:YA:2284:C:H41   | 52:Y6:25:LYS:NZ    | 2.15                     | 0.45              |
| 25:YA:2025:C:H2'   | 25:YA:2026:C:C6    | 2.52                     | 0.45              |
| 25:YA:2346:A:H8    | 54:Y8:35:GLN:HE21  | 1.64                     | 0.45              |
| 25:YA:2689:U:H4'   | 25:YA:2690:C:O5'   | 2.15                     | 0.45              |
| 25:YA:2630:G:O4'   | 25:YA:2894:G:H1'   | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:153:LYS:CB   | 31:YH:154:PRO:HD3  | 2.47                     | 0.45              |
| 31:YH:3:ARG:HA     | 31:YH:3:ARG:NE     | 2.32                     | 0.45              |
| 35:YP:126:VAL:HG12 | 35:YP:147:LEU:HD22 | 1.99                     | 0.45              |
| 26:YB:50:G:H5''    | 38:YS:61:ASN:ND2   | 2.32                     | 0.45              |
| 42:YW:97:LYS:HE2   | 42:YW:99:ARG:NH2   | 2.32                     | 0.45              |
| 45:YZ:82:ARG:HG3   | 45:YZ:83:PRO:CD    | 2.47                     | 0.45              |
| 45:YZ:94:GLU:HB2   | 45:YZ:95:PRO:HA    | 1.99                     | 0.45              |
| 1:QA:224:C:H2'     | 1:QA:225:C:H6      | 1.82                     | 0.44              |
| 1:QA:318:G:H2'     | 1:QA:319:G:C8      | 2.52                     | 0.44              |
| 1:QA:584:G:H2'     | 1:QA:585:G:H8      | 1.82                     | 0.44              |
| 2:QB:51:LEU:HD22   | 2:QB:55:PHE:HE2    | 1.82                     | 0.44              |
| 6:QF:41:GLU:HB3    | 6:QF:62:TRP:HB3    | 1.99                     | 0.44              |
| 10:QJ:40:LEU:HB2   | 10:QJ:69:ASN:CB    | 2.47                     | 0.44              |
| 19:QS:10:PHE:HB2   | 19:QS:39:THR:H     | 1.82                     | 0.44              |
| 47:R1:83:GLU:N     | 47:R1:83:GLU:OE2   | 2.49                     | 0.44              |
| 25:RA:2712:U:OP1   | 25:RA:2714:G:H4'   | 2.17                     | 0.44              |
| 27:RD:105:ILE:HD12 | 27:RD:105:ILE:HA   | 1.63                     | 0.44              |
| 34:RO:111:PHE:HB3  | 34:RO:114:ILE:HG13 | 1.98                     | 0.44              |
| 37:RR:29:LEU:HA    | 37:RR:29:LEU:HD12  | 1.74                     | 0.44              |
| 37:RR:28:LEU:HD12  | 37:RR:48:VAL:HG11  | 1.99                     | 0.44              |
| 44:RY:42:VAL:HG12  | 44:RY:65:ALA:HB3   | 1.99                     | 0.44              |
| 1:XA:1226:C:OP2    | 13:XM:103:THR:OG1  | 2.24                     | 0.44              |
| 1:XA:1517:G:H1'    | 25:YA:1919:A:O3'   | 2.17                     | 0.44              |
| 1:XA:312:C:H2'     | 1:XA:313:A:C8      | 2.52                     | 0.44              |
| 2:XB:33:TYR:HB2    | 2:XB:43:ASP:HB2    | 1.98                     | 0.44              |
| 8:XH:65:TYR:HA     | 8:XH:79:VAL:HG23   | 1.98                     | 0.44              |
| 11:XK:28:THR:OG1   | 11:XK:90:GLY:HA3   | 2.17                     | 0.44              |
| 10:XJ:61:GLU:OE1   | 14:XN:58:LYS:HE2   | 2.17                     | 0.44              |
| 47:Y1:53:VAL:HB    | 47:Y1:58:ILE:HD13  | 1.98                     | 0.44              |
| 35:YP:61:ARG:CD    | 54:Y8:13:ARG:HD2   | 2.46                     | 0.44              |
| 25:YA:1984:G:H2'   | 25:YA:1985:G:H8    | 1.82                     | 0.44              |
| 25:YA:270(J):G:H2' | 25:YA:270(K):C:O4' | 2.18                     | 0.44              |
| 27:YD:39:LYS:HB2   | 27:YD:62:TYR:HB2   | 1.98                     | 0.44              |
| 28:YE:167:VAL:HG21 | 28:YE:187:ALA:CB   | 2.47                     | 0.44              |
| 34:YO:86:ILE:HG22  | 34:YO:94:ARG:HD3   | 1.99                     | 0.44              |
| 1:QA:1105:A:H2'    | 1:QA:1106:G:C8     | 2.51                     | 0.44              |
| 1:QA:1336:C:H1'    | 1:QA:1337:G:C2     | 2.53                     | 0.44              |
| 1:QA:620:C:H2'     | 1:QA:621:A:O4'     | 2.18                     | 0.44              |
| 1:QA:992:U:H1'     | 1:QA:993:G:OP2     | 2.17                     | 0.44              |
| 2:QB:163:PHE:HA    | 2:QB:185:ILE:HG13  | 1.99                     | 0.44              |
| 2:QB:30:ARG:HH21   | 2:QB:194:PRO:HG2   | 1.81                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:QF:23:LYS:O     | 6:QF:27:GLN:HG2    | 2.17                     | 0.44              |
| 1:QA:1152:A:H5''  | 10:QJ:13:HIS:HD2   | 1.82                     | 0.44              |
| 19:QS:66:MET:HB2  | 19:QS:74:PHE:CZ    | 2.51                     | 0.44              |
| 1:QA:1222:G:OP1   | 19:QS:77:THR:HG21  | 2.17                     | 0.44              |
| 25:RA:188:G:H5'   | 47:R1:14:VAL:HG21  | 1.99                     | 0.44              |
| 25:RA:77:C:H5''   | 48:R2:10:LEU:HD11  | 1.97                     | 0.44              |
| 25:RA:2392:A:OP2  | 54:R8:31:HIS:HD2   | 1.99                     | 0.44              |
| 25:RA:1337:G:H2'  | 25:RA:1338:G:H8    | 1.81                     | 0.44              |
| 25:RA:1664:A:H61  | 25:RA:1996:C:H42   | 1.65                     | 0.44              |
| 31:RH:109:PHE:CZ  | 31:RH:152:ARG:HG2  | 2.53                     | 0.44              |
| 33:RN:114:ARG:O   | 33:RN:115:ARG:HB3  | 2.17                     | 0.44              |
| 34:RO:87:ILE:HD12 | 34:RO:91:LEU:HD12  | 1.99                     | 0.44              |
| 36:RQ:12:GLN:HE21 | 36:RQ:72:LYS:HD3   | 1.82                     | 0.44              |
| 1:XA:547:A:OP1    | 4:XD:73:ARG:NH2    | 2.49                     | 0.44              |
| 2:XB:12:GLU:C     | 2:XB:14:GLY:H      | 2.21                     | 0.44              |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HD13  | 1.98                     | 0.44              |
| 9:XI:95:LYS:HZ3   | 9:XI:96:LEU:HD13   | 1.83                     | 0.44              |
| 10:XJ:16:LEU:HD11 | 10:XJ:70:ARG:HB2   | 1.99                     | 0.44              |
| 12:XL:46:LYS:CG   | 12:XL:47:LYS:N     | 2.80                     | 0.44              |
| 13:XM:5:ALA:O     | 13:XM:7:VAL:N      | 2.49                     | 0.44              |
| 1:XA:1186:G:H21   | 14:XN:61:TRP:C     | 2.21                     | 0.44              |
| 21:XU:5:ASP:HB3   | 21:XU:8:THR:OG1    | 2.17                     | 0.44              |
| 23:XW:11:C:N4     | 23:XW:24:G:H1      | 2.15                     | 0.44              |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CG    | 2.48                     | 0.44              |
| 25:YA:1717:G:H1   | 25:YA:1742:C:H42   | 1.65                     | 0.44              |
| 25:YA:833:U:H2'   | 25:YA:834:C:C6     | 2.52                     | 0.44              |
| 25:YA:841:A:H2'   | 25:YA:842:G:C8     | 2.52                     | 0.44              |
| 42:YW:33:ARG:NH2  | 42:YW:52:GLU:OE1   | 2.50                     | 0.44              |
| 43:YX:35:THR:O    | 43:YX:39:ILE:HG13  | 2.16                     | 0.44              |
| 45:YZ:19:ARG:NH1  | 45:YZ:84:GLU:HB2   | 2.32                     | 0.44              |
| 1:QA:1053:G:O6    | 1:QA:1199:U:H2'    | 2.17                     | 0.44              |
| 1:QA:1350:A:OP2   | 9:QI:118:LYS:NZ    | 2.47                     | 0.44              |
| 1:QA:1372:U:H2'   | 1:QA:1373:G:O4'    | 2.18                     | 0.44              |
| 1:QA:20:U:O2      | 1:QA:916:G:C2      | 2.70                     | 0.44              |
| 52:R6:32:ASN:OD1  | 52:R6:32:ASN:N     | 2.49                     | 0.44              |
| 25:RA:2537:U:H2'  | 25:RA:2538:C:C6    | 2.53                     | 0.44              |
| 25:RA:300:A:H1'   | 25:RA:319:C:H1'    | 1.99                     | 0.44              |
| 25:RA:512:G:H4'   | 25:RA:513:A:O5'    | 2.18                     | 0.44              |
| 33:RN:116:LEU:HA  | 33:RN:116:LEU:HD23 | 1.78                     | 0.44              |
| 1:XA:1499:A:H1'   | 1:XA:1520:G:H5'    | 1.99                     | 0.44              |
| 4:XD:25:ARG:NH1   | 4:XD:30:LYS:HG3    | 2.32                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:XG:138:LYS:HE2  | 7:XG:142:GLU:OE2   | 2.17                     | 0.44              |
| 7:XG:87:VAL:HG11  | 7:XG:155:ARG:HA    | 1.99                     | 0.44              |
| 8:XH:83:ILE:HB    | 8:XH:137:VAL:HG13  | 1.99                     | 0.44              |
| 8:XH:51:VAL:HG11  | 8:XH:60:ARG:HG3    | 1.99                     | 0.44              |
| 25:YA:517:C:OP1   | 51:Y5:16:ARG:NH2   | 2.49                     | 0.44              |
| 25:YA:1165:U:H2'  | 25:YA:1166:C:C6    | 2.53                     | 0.44              |
| 25:YA:858:U:H1'   | 25:YA:2268:A:H2'   | 2.00                     | 0.44              |
| 25:YA:2356:C:H2'  | 25:YA:2357:U:O4'   | 2.18                     | 0.44              |
| 25:YA:2470:G:H5'  | 36:YQ:56:ARG:NH2   | 2.30                     | 0.44              |
| 25:YA:2784:C:O2'  | 28:YE:37:ARG:NH1   | 2.50                     | 0.44              |
| 25:YA:279:C:H42   | 25:YA:361:G:H1     | 1.65                     | 0.44              |
| 26:YB:15:A:H5'    | 26:YB:16:G:H8      | 1.82                     | 0.44              |
| 30:YG:114:ILE:HB  | 30:YG:117:PHE:HB2  | 1.99                     | 0.44              |
| 31:YH:52:VAL:HG21 | 31:YH:68:THR:HG22  | 2.00                     | 0.44              |
| 33:YN:62:VAL:HG12 | 33:YN:66:LYS:HD2   | 1.98                     | 0.44              |
| 34:YO:17:ARG:NH2  | 34:YO:47:ILE:HD13  | 2.33                     | 0.44              |
| 40:YU:104:GLN:OE1 | 40:YU:105:VAL:HG23 | 2.18                     | 0.44              |
| 40:YU:66:ASN:HB2  | 40:YU:76:TYR:HB2   | 1.99                     | 0.44              |
| 41:YV:99:ILE:H    | 41:YV:99:ILE:HD13  | 1.82                     | 0.44              |
| 1:QA:1439:C:H42   | 1:QA:1462:G:H1     | 1.63                     | 0.44              |
| 1:QA:601:C:H2'    | 1:QA:602:A:C8      | 2.53                     | 0.44              |
| 1:QA:974:A:H1'    | 14:QN:31:ARG:NE    | 2.31                     | 0.44              |
| 1:QA:1191:A:P     | 3:QC:3:ASN:HD22    | 2.41                     | 0.44              |
| 10:QJ:33:GLN:O    | 10:QJ:75:ILE:HG12  | 2.17                     | 0.44              |
| 20:QT:16:HIS:O    | 20:QT:19:SER:HB3   | 2.17                     | 0.44              |
| 1:QA:1305:G:H5'   | 21:QU:4:GLY:HA3    | 1.99                     | 0.44              |
| 25:RA:144:C:H2'   | 25:RA:145:G:H8     | 1.82                     | 0.44              |
| 25:RA:1537:C:H2'  | 25:RA:1538:G:C8    | 2.52                     | 0.44              |
| 27:RD:49:ILE:CD1  | 27:RD:52:ARG:HA    | 2.47                     | 0.44              |
| 30:RG:51:ARG:O    | 30:RG:53:LEU:N     | 2.48                     | 0.44              |
| 30:RG:57:ALA:HB1  | 30:RG:68:PRO:HG2   | 1.99                     | 0.44              |
| 35:RP:140:ALA:O   | 35:RP:141:ALA:HB2  | 2.17                     | 0.44              |
| 39:RT:36:GLU:HG3  | 39:RT:41:ARG:CD    | 2.45                     | 0.44              |
| 40:RU:65:ILE:HG12 | 40:RU:96:ALA:CB    | 2.47                     | 0.44              |
| 43:RX:53:LYS:NZ   | 43:RX:55:ASN:HD21  | 2.15                     | 0.44              |
| 45:RZ:103:ARG:HD3 | 45:RZ:136:PHE:CD2  | 2.53                     | 0.44              |
| 4:XD:50:ARG:HG3   | 4:XD:50:ARG:H      | 1.63                     | 0.44              |
| 12:XL:24:VAL:O    | 12:XL:26:ALA:N     | 2.47                     | 0.44              |
| 20:XT:87:LYS:O    | 20:XT:91:LEU:HG    | 2.17                     | 0.44              |
| 22:XV:53:G:H4'    | 22:XV:54:U:OP1     | 2.17                     | 0.44              |
| 25:YA:1087:G:C4   | 25:YA:1089:G:H1'   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 25:YA:1981:A:H5'' | 25:YA:1982:C:OP2    | 2.17                     | 0.44              |
| 25:YA:2293:C:OP1  | 38:YS:89:ARG:NH1    | 2.51                     | 0.44              |
| 27:YD:248:SER:HB2 | 27:YD:252:TRP:CZ2   | 2.51                     | 0.44              |
| 29:YF:63:LYS:HE3  | 29:YF:65:TRP:O      | 2.18                     | 0.44              |
| 33:YN:134:ARG:O   | 33:YN:136:GLU:N     | 2.50                     | 0.44              |
| 4:QD:150:GLU:OE1  | 4:QD:150:GLU:N      | 2.51                     | 0.44              |
| 5:QE:97:GLY:N     | 5:QE:117:ASP:OD2    | 2.40                     | 0.44              |
| 16:QP:23:ASP:O    | 16:QP:26:ARG:HB2    | 2.17                     | 0.44              |
| 51:R5:55:ARG:NH1  | 51:R5:55:ARG:HG2    | 2.33                     | 0.44              |
| 25:RA:2821:A:OP2  | 25:RA:2822:G:OP2    | 2.36                     | 0.44              |
| 26:RB:24:G:H1'    | 26:RB:27:C:N4       | 2.33                     | 0.44              |
| 30:RG:37:VAL:O    | 30:RG:94:LEU:HG     | 2.17                     | 0.44              |
| 38:RS:11:LYS:HG3  | 38:RS:91:PRO:HD3    | 1.98                     | 0.44              |
| 41:RV:16:PRO:HB3  | 41:RV:97:LYS:O      | 2.17                     | 0.44              |
| 1:XA:1004:A:H1'   | 1:XA:1036:G:N2      | 2.28                     | 0.44              |
| 1:XA:1221:G:O3'   | 19:XS:77:THR:HG21   | 2.16                     | 0.44              |
| 1:XA:1417:G:C6    | 1:XA:1482:G:C6      | 3.06                     | 0.44              |
| 1:XA:321:A:N6     | 1:XA:329:A:OP2      | 2.50                     | 0.44              |
| 1:XA:97:U:H2'     | 1:XA:99:C:C6        | 2.52                     | 0.44              |
| 1:XA:963:G:H21    | 10:XJ:55:LYS:HD3    | 1.81                     | 0.44              |
| 15:XO:32:LEU:O    | 15:XO:36:ILE:HG13   | 2.18                     | 0.44              |
| 23:XW:9:A:O4'     | 23:XW:46:G:N2       | 2.51                     | 0.44              |
| 52:Y6:34:LEU:H    | 52:Y6:34:LEU:HD13   | 1.82                     | 0.44              |
| 52:Y6:41:PRO:HD2  | 52:Y6:46:HIS:H      | 1.81                     | 0.44              |
| 25:YA:1021:A:N6   | 25:YA:1142(A):A:H61 | 2.03                     | 0.44              |
| 25:YA:1434:A:H61  | 25:YA:1558:A:N6     | 2.15                     | 0.44              |
| 25:YA:1543:A:O2'  | 25:YA:1544:C:OP2    | 2.31                     | 0.44              |
| 29:YF:47:GLY:HA3  | 29:YF:95:ARG:O      | 2.18                     | 0.44              |
| 25:YA:2667:C:H1'  | 31:YH:109:PHE:HD1   | 1.82                     | 0.44              |
| 39:YT:61:PHE:CE1  | 39:YT:76:PHE:HB2    | 2.53                     | 0.44              |
| 39:YT:42:ILE:HG21 | 39:YT:84:GLN:NE2    | 2.32                     | 0.44              |
| 40:YU:88:ILE:H    | 40:YU:88:ILE:HG12   | 1.49                     | 0.44              |
| 44:YY:51:VAL:O    | 44:YY:56:PRO:HA     | 2.18                     | 0.44              |
| 45:YZ:19:ARG:HD3  | 45:YZ:25:PRO:HD2    | 1.99                     | 0.44              |
| 1:QA:1111:A:N1    | 3:QC:177:THR:OG1    | 2.43                     | 0.44              |
| 1:QA:1277:C:O2'   | 1:QA:1279:A:H8      | 2.01                     | 0.44              |
| 1:QA:966:G:O2'    | 9:QI:127:LYS:O      | 2.35                     | 0.44              |
| 20:QT:87:LYS:HA   | 20:QT:87:LYS:HD2    | 1.68                     | 0.44              |
| 22:QV:15:C:O2'    | 22:QV:61:C:OP1      | 2.36                     | 0.44              |
| 48:R2:49:LYS:O    | 48:R2:53:LEU:HB2    | 2.18                     | 0.44              |
| 25:RA:1085:A:HO2' | 25:RA:1086:A:P      | 2.40                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1534:G:H2'   | 25:RA:1534:G:N3    | 2.32                     | 0.44              |
| 27:RD:70:TRP:HZ3   | 27:RD:146:GLU:OE2  | 2.01                     | 0.44              |
| 27:RD:34:VAL:HG22  | 27:RD:35:LYS:HG3   | 2.00                     | 0.44              |
| 29:RF:117:ARG:HH12 | 35:RP:1:MET:N      | 2.16                     | 0.44              |
| 32:RI:93:THR:H     | 32:RI:96:ASP:HB2   | 1.82                     | 0.44              |
| 25:RA:1007:C:H5"   | 33:RN:35:ARG:HH11  | 1.81                     | 0.44              |
| 34:RO:22:ILE:HA    | 34:RO:22:ILE:HD13  | 1.77                     | 0.44              |
| 35:RP:37:GLY:O     | 35:RP:40:SER:OG    | 2.27                     | 0.44              |
| 41:RV:49:THR:HB    | 41:RV:50:PRO:HD2   | 1.99                     | 0.44              |
| 25:RA:748:G:C8     | 42:RW:89:ALA:HB1   | 2.53                     | 0.44              |
| 1:XA:485:G:H1'     | 1:XA:486:U:H5      | 1.83                     | 0.44              |
| 1:XA:582:U:H2'     | 1:XA:583:A:H8      | 1.81                     | 0.44              |
| 1:XA:636:U:H2'     | 1:XA:637:G:H8      | 1.82                     | 0.44              |
| 1:XA:701:C:O2      | 1:XA:703:G:N1      | 2.50                     | 0.44              |
| 3:XC:47:LEU:HA     | 3:XC:47:LEU:HD12   | 1.83                     | 0.44              |
| 1:XA:1190:G:OP1    | 3:XC:4:LYS:HA      | 2.17                     | 0.44              |
| 3:XC:82:GLU:O      | 3:XC:86:VAL:HG13   | 2.17                     | 0.44              |
| 12:XL:78:GLN:HB3   | 12:XL:79:GLU:H     | 1.67                     | 0.44              |
| 15:XO:26:GLU:HG2   | 15:XO:26:GLU:H     | 1.54                     | 0.44              |
| 18:XR:52:PRO:HB2   | 18:XR:54:ARG:HG2   | 2.00                     | 0.44              |
| 48:Y2:17:SER:CB    | 48:Y2:67:LYS:HE3   | 2.47                     | 0.44              |
| 52:Y6:7:ILE:HD12   | 52:Y6:7:ILE:HA     | 1.85                     | 0.44              |
| 25:YA:1019:U:HO2'  | 25:YA:1021:A:H2    | 1.60                     | 0.44              |
| 25:YA:1332:G:H8    | 25:YA:1332:G:H2'   | 1.67                     | 0.44              |
| 25:YA:1535:U:H5"   | 25:YA:1537:C:C4    | 2.52                     | 0.44              |
| 25:YA:2756:U:H1'   | 25:YA:2757:A:H5"   | 2.00                     | 0.44              |
| 25:YA:2627:G:O2'   | 25:YA:2781:A:N1    | 2.41                     | 0.44              |
| 25:YA:2811:G:H1    | 25:YA:2889:C:H42   | 1.65                     | 0.44              |
| 25:YA:455:C:HO2'   | 25:YA:472:A:H2     | 1.64                     | 0.44              |
| 25:YA:653:A:H4'    | 25:YA:654:A:OP2    | 2.18                     | 0.44              |
| 25:YA:839:U:H2'    | 25:YA:840:C:C6     | 2.53                     | 0.44              |
| 26:YB:3:C:H2'      | 26:YB:4:C:C6       | 2.52                     | 0.44              |
| 27:YD:85:ASP:HB2   | 27:YD:92:ILE:HD13  | 1.99                     | 0.44              |
| 30:YG:47:LYS:HB2   | 30:YG:47:LYS:HE3   | 1.73                     | 0.44              |
| 30:YG:98:ARG:O     | 30:YG:101:ILE:HG13 | 2.17                     | 0.44              |
| 31:YH:124:GLU:HB3  | 31:YH:132:ARG:HG3  | 1.99                     | 0.44              |
| 41:YV:15:GLU:HG3   | 41:YV:16:PRO:HD2   | 1.99                     | 0.44              |
| 43:YX:70:LEU:H     | 43:YX:70:LEU:HD23  | 1.83                     | 0.44              |
| 45:YZ:80:ARG:NH2   | 45:YZ:82:ARG:HH22  | 2.12                     | 0.44              |
| 1:QA:1244:C:H42    | 1:QA:1293:G:H1     | 1.65                     | 0.44              |
| 1:QA:297:G:N2      | 1:QA:300:A:OP2     | 2.48                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:484:G:H4'     | 1:QA:485:G:O5'    | 2.16                     | 0.44              |
| 3:QC:70:VAL:HG21   | 3:QC:76:VAL:HG11  | 2.00                     | 0.44              |
| 7:QG:113:GLU:HG2   | 7:QG:113:GLU:H    | 1.39                     | 0.44              |
| 10:QJ:51:ARG:NE    | 10:QJ:60:ARG:O    | 2.45                     | 0.44              |
| 10:QJ:47:PHE:HE1   | 10:QJ:63:PHE:HB2  | 1.83                     | 0.44              |
| 15:QO:50:HIS:O     | 15:QO:53:HIS:HB3  | 2.17                     | 0.44              |
| 22:QV:43:A:H2'     | 22:QV:44:A:C8     | 2.53                     | 0.44              |
| 55:R9:24:TYR:CE2   | 55:R9:35:ARG:HG3  | 2.53                     | 0.44              |
| 25:RA:2563:U:H4'   | 34:RO:28:SER:HA   | 2.00                     | 0.44              |
| 25:RA:271(B):G:H2' | 25:RA:421:U:OP2   | 2.17                     | 0.44              |
| 29:RF:9:ILE:HA     | 29:RF:10:PRO:HD3  | 1.89                     | 0.44              |
| 30:RG:171:ALA:O    | 30:RG:175:LEU:HG  | 2.18                     | 0.44              |
| 31:RH:28:GLY:HA3   | 31:RH:79:VAL:HB   | 2.00                     | 0.44              |
| 38:RS:19:LYS:O     | 38:RS:20:ARG:HB3  | 2.17                     | 0.44              |
| 41:RV:35:LEU:CD2   | 41:RV:57:VAL:HG22 | 2.47                     | 0.44              |
| 45:RZ:102:LEU:HB3  | 45:RZ:104:PHE:CE1 | 2.52                     | 0.44              |
| 45:RZ:148:ASP:OD1  | 45:RZ:149:SER:N   | 2.50                     | 0.44              |
| 1:XA:1399:C:C2     | 1:XA:1401:G:C5    | 3.06                     | 0.44              |
| 1:XA:64:G:N2       | 1:XA:68:G:O6      | 2.42                     | 0.44              |
| 4:XD:153:ARG:NH1   | 4:XD:181:MET:HB2  | 2.32                     | 0.44              |
| 6:XF:33:TYR:HB2    | 6:XF:75:LEU:HD12  | 1.99                     | 0.44              |
| 2:XB:195:ASP:O     | 8:XH:74:PRO:HG3   | 2.18                     | 0.44              |
| 12:XL:42:THR:HA    | 12:XL:53:ARG:O    | 2.18                     | 0.44              |
| 15:XO:77:ARG:HA    | 15:XO:80:ALA:HB3  | 1.99                     | 0.44              |
| 15:XO:82:ILE:O     | 15:XO:86:GLY:N    | 2.51                     | 0.44              |
| 16:XP:18:ARG:NH1   | 16:XP:32:TYR:OH   | 2.50                     | 0.44              |
| 19:XS:81:ARG:HB2   | 19:XS:81:ARG:HE   | 1.36                     | 0.44              |
| 50:Y4:35:VAL:C     | 50:Y4:37:SER:H    | 2.20                     | 0.44              |
| 25:YA:1183:G:H4'   | 49:Y3:29:ARG:HH22 | 1.82                     | 0.44              |
| 25:YA:1608:A:H1'   | 25:YA:1610:A:OP2  | 2.17                     | 0.44              |
| 25:YA:1914:C:H2'   | 25:YA:1915:U:O4'  | 2.18                     | 0.44              |
| 25:YA:2347:C:H2'   | 25:YA:2348:U:H6   | 1.83                     | 0.44              |
| 25:YA:627:A:H4'    | 25:YA:628:G:H5'   | 1.99                     | 0.44              |
| 26:YB:24:G:H5''    | 26:YB:25:A:OP1    | 2.17                     | 0.44              |
| 32:YI:88:ILE:HG12  | 32:YI:122:GLU:H   | 1.83                     | 0.44              |
| 39:YT:48:ILE:H     | 39:YT:48:ILE:HD12 | 1.83                     | 0.44              |
| 45:YZ:52:SER:O     | 45:YZ:54:HIS:N    | 2.50                     | 0.44              |
| 1:QA:584:G:H2'     | 1:QA:585:G:C8     | 2.53                     | 0.44              |
| 1:QA:991:U:O2      | 1:QA:993:G:H8     | 2.01                     | 0.44              |
| 2:QB:71:VAL:HA     | 2:QB:93:VAL:HB    | 2.00                     | 0.44              |
| 7:QG:116:ALA:HA    | 7:QG:119:ARG:HE   | 1.83                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:QK:92:GLU:HB3  | 11:QK:96:ARG:NH1   | 2.33                     | 0.44              |
| 23:QW:19:G:H22    | 23:QW:56:C:N4      | 2.16                     | 0.44              |
| 25:RA:2396:G:O5'  | 47:R1:25:LYS:HE2   | 2.18                     | 0.44              |
| 51:R5:16:ARG:HD2  | 51:R5:20:ARG:NH1   | 2.33                     | 0.44              |
| 51:R5:59:GLU:H    | 51:R5:59:GLU:HG2   | 1.64                     | 0.44              |
| 25:RA:1331:A:O2'  | 25:RA:1332:G:H8    | 2.00                     | 0.44              |
| 25:RA:1543:A:H2   | 25:RA:1545:A:N7    | 2.16                     | 0.44              |
| 25:RA:807:U:O2'   | 25:RA:2060:A:N1    | 2.46                     | 0.44              |
| 30:RG:95:ARG:O    | 30:RG:99:MET:HG2   | 2.18                     | 0.44              |
| 31:RH:123:PHE:O   | 31:RH:125:VAL:HG23 | 2.18                     | 0.44              |
| 25:RA:558:G:OP1   | 33:RN:111:PRO:HD2  | 2.18                     | 0.44              |
| 37:RR:54:LEU:HD23 | 37:RR:66:VAL:HG23  | 1.98                     | 0.44              |
| 39:RT:107:ASP:O   | 39:RT:111:ARG:NH1  | 2.51                     | 0.44              |
| 43:RX:57:LEU:HD11 | 43:RX:78:LYS:HD2   | 1.99                     | 0.44              |
| 43:RX:87:GLN:O    | 43:RX:88:LYS:HG3   | 2.18                     | 0.44              |
| 1:XA:1124:G:H3'   | 1:XA:1145:C:H41    | 1.83                     | 0.44              |
| 1:XA:690:G:H22    | 11:XK:55:LYS:HZ1   | 1.66                     | 0.44              |
| 1:XA:939:G:H5''   | 7:XG:102:ARG:NH2   | 2.32                     | 0.44              |
| 12:XL:39:VAL:HG12 | 12:XL:41:ARG:HG3   | 2.00                     | 0.44              |
| 46:Y0:43:THR:HG23 | 46:Y0:43:THR:O     | 2.17                     | 0.44              |
| 48:Y2:31:GLU:HB2  | 48:Y2:53:LEU:HD11  | 2.00                     | 0.44              |
| 19:XS:64:GLU:HG3  | 50:Y4:55:ARG:HH12  | 1.81                     | 0.44              |
| 54:Y8:49:VAL:HG23 | 54:Y8:53:PRO:HB3   | 2.00                     | 0.44              |
| 25:YA:18:C:O2'    | 25:YA:553:U:OP1    | 2.35                     | 0.44              |
| 26:YB:80:U:O2'    | 26:YB:81:G:H5'     | 2.18                     | 0.44              |
| 25:YA:2619:C:H5'' | 28:YE:152:LYS:HA   | 1.99                     | 0.44              |
| 28:YE:37:ARG:O    | 28:YE:45:THR:HA    | 2.18                     | 0.44              |
| 45:YZ:166:SER:HB2 | 45:YZ:167:PRO:C    | 2.39                     | 0.44              |
| 1:QA:1015:A:H1'   | 1:QA:1219:U:H5'    | 2.00                     | 0.44              |
| 1:QA:1231:G:O3'   | 9:QI:126:SER:OG    | 2.22                     | 0.44              |
| 1:QA:17:U:H2'     | 1:QA:18:C:C6       | 2.53                     | 0.44              |
| 1:QA:280:C:H3'    | 1:QA:281:G:H5'     | 1.99                     | 0.44              |
| 1:QA:489:C:H2'    | 1:QA:490:G:H8      | 1.83                     | 0.44              |
| 1:QA:738:C:OP2    | 6:QF:92:LYS:NZ     | 2.50                     | 0.44              |
| 1:QA:900:A:H2'    | 1:QA:901:A:C8      | 2.53                     | 0.44              |
| 1:QA:936:C:H2'    | 1:QA:937:A:O4'     | 2.18                     | 0.44              |
| 1:QA:97:U:H2'     | 1:QA:99:C:C6       | 2.53                     | 0.44              |
| 2:QB:228:GLY:O    | 2:QB:230:VAL:N     | 2.50                     | 0.44              |
| 12:QL:44:THR:HA   | 12:QL:45:PRO:HD3   | 1.74                     | 0.44              |
| 15:QO:39:LEU:HD23 | 15:QO:39:LEU:HA    | 1.68                     | 0.44              |
| 52:R6:40:CYS:HA   | 52:R6:41:PRO:HD2   | 1.85                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1178:C:H2'   | 25:RA:1179:C:C6   | 2.53                     | 0.44              |
| 25:RA:134:C:H2'    | 25:RA:135:G:C8    | 2.53                     | 0.44              |
| 25:RA:191:A:H2'    | 25:RA:192:C:C6    | 2.52                     | 0.44              |
| 25:RA:2556:C:H2'   | 25:RA:2557:G:O4'  | 2.17                     | 0.44              |
| 25:RA:859:G:O2'    | 25:RA:860:U:O2    | 2.20                     | 0.44              |
| 27:RD:65:ILE:H     | 27:RD:65:ILE:HD13 | 1.82                     | 0.44              |
| 28:RE:143:ASN:HD22 | 28:RE:147:PRO:HD3 | 1.83                     | 0.44              |
| 30:RG:95:ARG:C     | 30:RG:99:MET:HG2  | 2.38                     | 0.44              |
| 32:RI:64:GLU:O     | 32:RI:67:ARG:NH2  | 2.51                     | 0.44              |
| 37:RR:27:SER:HB3   | 37:RR:34:ILE:HD11 | 2.00                     | 0.44              |
| 45:RZ:29:TYR:CE2   | 45:RZ:87:ASP:HB3  | 2.53                     | 0.44              |
| 1:XA:130:A:N3      | 1:XA:263:A:O2'    | 2.43                     | 0.44              |
| 1:XA:606:G:N2      | 1:XA:631:G:H8     | 2.16                     | 0.44              |
| 1:XA:791:G:H2'     | 1:XA:792:A:H5'    | 2.00                     | 0.44              |
| 12:XL:62:SER:C     | 12:XL:64:TYR:H    | 2.21                     | 0.44              |
| 13:XM:23:TYR:HE2   | 13:XM:70:LEU:HD12 | 1.83                     | 0.44              |
| 47:Y1:70:VAL:O     | 47:Y1:73:LEU:HB2  | 2.18                     | 0.44              |
| 50:Y4:48:ARG:CZ    | 50:Y4:51:ASP:HA   | 2.47                     | 0.44              |
| 50:Y4:60:GLN:HB3   | 50:Y4:61:ARG:H    | 1.55                     | 0.44              |
| 13:XM:80:ARG:NE    | 50:Y4:71:ARG:HH22 | 2.12                     | 0.44              |
| 25:YA:2114:A:H3'   | 25:YA:2114:A:N3   | 2.32                     | 0.44              |
| 25:YA:414:C:H2'    | 25:YA:415:A:C8    | 2.53                     | 0.44              |
| 28:YE:105:THR:OG1  | 28:YE:199:ARG:NH1 | 2.50                     | 0.44              |
| 29:YF:184:TYR:CE2  | 29:YF:188:ARG:HD2 | 2.52                     | 0.44              |
| 31:YH:4:ILE:H      | 31:YH:4:ILE:HG12  | 1.59                     | 0.44              |
| 1:QA:838:G:C6      | 1:QA:842:C:H1'    | 2.53                     | 0.43              |
| 2:QB:74:LYS:O      | 2:QB:78:GLN:HG3   | 2.18                     | 0.43              |
| 17:QQ:60:ILE:HB    | 17:QQ:74:LEU:HD23 | 2.00                     | 0.43              |
| 52:R6:41:PRO:HD2   | 52:R6:46:HIS:H    | 1.83                     | 0.43              |
| 25:RA:1363:C:H2'   | 25:RA:1364:G:H8   | 1.83                     | 0.43              |
| 25:RA:1543:A:N3    | 25:RA:1545:A:O4'  | 2.51                     | 0.43              |
| 25:RA:210:C:H2'    | 25:RA:211:A:C8    | 2.53                     | 0.43              |
| 27:RD:72:LYS:NZ    | 27:RD:99:ASP:OD2  | 2.43                     | 0.43              |
| 28:RE:119:ARG:HD3  | 28:RE:160:TYR:HB2 | 2.00                     | 0.43              |
| 44:RY:81:LYS:HB2   | 44:RY:96:ILE:CG2  | 2.48                     | 0.43              |
| 1:XA:1147:C:O2     | 9:XI:16:ARG:NH1   | 2.51                     | 0.43              |
| 1:XA:793:U:H3'     | 1:XA:794:A:H5''   | 1.99                     | 0.43              |
| 3:XC:108:ASN:HB3   | 3:XC:111:LEU:HD12 | 2.00                     | 0.43              |
| 11:XK:19:ALA:HB2   | 11:XK:32:ILE:HG22 | 2.00                     | 0.43              |
| 15:XO:39:LEU:HD13  | 15:XO:56:LEU:HB2  | 2.00                     | 0.43              |
| 16:XP:39:TYR:CZ    | 16:XP:41:PRO:HB3  | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:XP:4:ILE:HB     | 16:XP:66:PRO:HB3   | 2.00                     | 0.43              |
| 25:YA:2271:G:OP1   | 46:Y0:18:ALA:HB1   | 2.17                     | 0.43              |
| 55:Y9:1:MET:O      | 55:Y9:34:GLN:HG2   | 2.18                     | 0.43              |
| 25:YA:1050:A:H8    | 25:YA:2751:G:O2'   | 2.01                     | 0.43              |
| 25:YA:2556:C:H2'   | 25:YA:2557:G:O4'   | 2.17                     | 0.43              |
| 25:YA:2566:A:H4'   | 25:YA:2567:G:O5'   | 2.18                     | 0.43              |
| 27:YD:250:TRP:HE3  | 27:YD:252:TRP:NE1  | 2.16                     | 0.43              |
| 27:YD:61:LEU:HA    | 27:YD:61:LEU:HD13  | 1.92                     | 0.43              |
| 28:YE:188:VAL:O    | 28:YE:188:VAL:HG13 | 2.18                     | 0.43              |
| 29:YF:66:PRO:O     | 29:YF:68:LYS:N     | 2.51                     | 0.43              |
| 30:YG:10:LYS:HE2   | 30:YG:175:LEU:O    | 2.18                     | 0.43              |
| 30:YG:67:LYS:HD2   | 30:YG:67:LYS:O     | 2.17                     | 0.43              |
| 26:YB:41:U:O4      | 30:YG:70:VAL:HG23  | 2.17                     | 0.43              |
| 31:YH:15:VAL:O     | 31:YH:15:VAL:HG23  | 2.17                     | 0.43              |
| 37:YR:38:VAL:HG22  | 37:YR:112:ALA:HB2  | 1.99                     | 0.43              |
| 1:QA:1124:G:H5''   | 1:QA:1145:C:H41    | 1.81                     | 0.43              |
| 1:QA:1200:C:O2'    | 1:QA:1201:A:OP2    | 2.29                     | 0.43              |
| 1:QA:1317:C:N3     | 19:QS:37:ARG:NH2   | 2.66                     | 0.43              |
| 1:QA:1488:G:H2'    | 1:QA:1489:G:H8     | 1.81                     | 0.43              |
| 1:QA:952:U:H2'     | 1:QA:953:G:H8      | 1.82                     | 0.43              |
| 3:QC:81:GLY:O      | 3:QC:85:ARG:HB2    | 2.18                     | 0.43              |
| 7:QG:9:VAL:HG13    | 7:QG:94:ARG:NH2    | 2.27                     | 0.43              |
| 9:QI:16:ARG:O      | 9:QI:63:ILE:HA     | 2.17                     | 0.43              |
| 12:QL:70:ILE:HD13  | 12:QL:77:LEU:HD12  | 1.99                     | 0.43              |
| 15:QO:17:ARG:HD3   | 15:QO:26:GLU:HG3   | 1.99                     | 0.43              |
| 47:R1:49:VAL:HG11  | 47:R1:70:VAL:HG11  | 1.98                     | 0.43              |
| 52:R6:28:ARG:HG3   | 52:R6:31:PRO:HD2   | 2.00                     | 0.43              |
| 25:RA:1497:U:H5''  | 25:RA:1498:C:H5    | 1.83                     | 0.43              |
| 25:RA:2102:U:H2'   | 25:RA:2103:C:C6    | 2.54                     | 0.43              |
| 25:RA:582:G:H2'    | 25:RA:583:G:C8     | 2.53                     | 0.43              |
| 28:RE:36:ARG:HH21  | 28:RE:88:GLY:HA2   | 1.84                     | 0.43              |
| 25:RA:2303:G:O2'   | 30:RG:132:ASN:HB2  | 2.17                     | 0.43              |
| 34:RO:106:LEU:HD23 | 34:RO:106:LEU:HA   | 1.81                     | 0.43              |
| 25:RA:2406:U:N3    | 35:RP:73:GLY:O     | 2.48                     | 0.43              |
| 36:RQ:136:ALA:O    | 36:RQ:138:ASP:N    | 2.46                     | 0.43              |
| 36:RQ:79:LEU:HA    | 36:RQ:79:LEU:HD22  | 1.82                     | 0.43              |
| 25:RA:2293:C:H5''  | 38:RS:89:ARG:HH12  | 1.84                     | 0.43              |
| 43:RX:67:GLY:O     | 43:RX:69:TYR:N     | 2.43                     | 0.43              |
| 1:XA:1062:U:H2'    | 1:XA:1063:C:C6     | 2.53                     | 0.43              |
| 1:XA:501:C:H1'     | 1:XA:549:C:H1'     | 2.00                     | 0.43              |
| 4:XD:112:VAL:N     | 4:XD:116:GLN:OE1   | 2.38                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:XD:100:ARG:NH1   | 4:XD:137:SER:HB3   | 2.33                     | 0.43              |
| 9:XI:118:LYS:O     | 9:XI:119:ALA:HB3   | 2.18                     | 0.43              |
| 13:XM:14:ARG:H     | 13:XM:44:ARG:CD    | 2.25                     | 0.43              |
| 35:YP:126:VAL:HG12 | 35:YP:147:LEU:CD2  | 2.48                     | 0.43              |
| 37:YR:34:ILE:HD13  | 37:YR:34:ILE:HA    | 1.71                     | 0.43              |
| 39:YT:35:LYS:H     | 39:YT:35:LYS:HD2   | 1.83                     | 0.43              |
| 41:YV:52:VAL:O     | 41:YV:54:GLY:N     | 2.51                     | 0.43              |
| 1:QA:1510:U:H2'    | 1:QA:1511:G:C8     | 2.52                     | 0.43              |
| 5:QE:100:VAL:HG22  | 5:QE:118:ILE:HG22  | 1.99                     | 0.43              |
| 1:QA:585:G:O3'     | 17:QQ:34:LYS:NZ    | 2.51                     | 0.43              |
| 25:RA:2226:C:H2'   | 25:RA:2227:A:O4'   | 2.18                     | 0.43              |
| 25:RA:2232:U:OP2   | 47:R1:40:ARG:NH1   | 2.42                     | 0.43              |
| 25:RA:2306:C:H2'   | 25:RA:2307:G:H21   | 1.83                     | 0.43              |
| 25:RA:270(F):U:H2' | 25:RA:270(G):C:C6  | 2.53                     | 0.43              |
| 27:RD:145:VAL:HG11 | 27:RD:175:LEU:HD11 | 2.00                     | 0.43              |
| 32:RI:124:GLY:O    | 32:RI:142:VAL:HG23 | 2.18                     | 0.43              |
| 44:RY:97:ARG:HE    | 44:RY:98:VAL:HB    | 1.83                     | 0.43              |
| 1:XA:1292:U:OP1    | 7:XG:41:ARG:NH2    | 2.51                     | 0.43              |
| 3:XC:72:LYS:HB3    | 3:XC:75:VAL:HG23   | 2.00                     | 0.43              |
| 10:XJ:32:ALA:H     | 10:XJ:78:ASN:ND2   | 2.16                     | 0.43              |
| 14:YN:29:ARG:HD3   | 14:YN:40:CYS:HB2   | 1.99                     | 0.43              |
| 15:XO:56:LEU:HD21  | 25:YA:715:G:C4     | 2.53                     | 0.43              |
| 25:YA:242:G:H3'    | 54:Y8:6:THR:HG23   | 1.99                     | 0.43              |
| 25:YA:2328:A:H2'   | 25:YA:2329:G:C8    | 2.53                     | 0.43              |
| 25:YA:898:C:C2'    | 25:YA:899:A:H5'    | 2.48                     | 0.43              |
| 31:YH:67:LEU:O     | 31:YH:71:LEU:HB2   | 2.17                     | 0.43              |
| 32:YI:130:TYR:N    | 32:YI:136:VAL:O    | 2.51                     | 0.43              |
| 37:YR:70:LEU:HA    | 37:YR:70:LEU:HD23  | 1.84                     | 0.43              |
| 56:Z7:1:T17:H66    | 56:Z7:2:GLY:N      | 2.21                     | 0.43              |
| 4:QD:171:GLY:HA2   | 4:QD:172:PRO:HD3   | 1.87                     | 0.43              |
| 9:QI:116:LYS:HE2   | 9:QI:122:ALA:HB2   | 2.01                     | 0.43              |
| 11:QK:19:ALA:HB2   | 11:QK:32:ILE:HG22  | 2.00                     | 0.43              |
| 11:QK:38:ASN:HA    | 11:QK:39:PRO:HD3   | 1.88                     | 0.43              |
| 17:QQ:63:ARG:HG2   | 17:QQ:64:PRO:HD2   | 2.00                     | 0.43              |
| 18:QR:37:VAL:HG22  | 18:QR:78:LEU:HB3   | 2.00                     | 0.43              |
| 22:QV:28:C:H2'     | 22:QV:29:G:H8      | 1.83                     | 0.43              |
| 25:RA:476:G:H1'    | 25:RA:480:A:N6     | 2.34                     | 0.43              |
| 25:RA:556:G:O5'    | 25:RA:556:G:H8     | 2.00                     | 0.43              |
| 25:RA:974(A):C:H4' | 25:RA:975:G:C5'    | 2.49                     | 0.43              |
| 33:RN:33:LEU:HA    | 33:RN:38:HIS:CE1   | 2.54                     | 0.43              |
| 33:RN:58:ASP:HB3   | 33:RN:95:PRO:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:RS:29:PHE:HD1  | 38:RS:92:TYR:HH    | 1.66                     | 0.43              |
| 44:RY:42:VAL:O    | 44:RY:65:ALA:N     | 2.45                     | 0.43              |
| 26:RB:75:G:H4'    | 45:RZ:36:LYS:HG2   | 2.00                     | 0.43              |
| 1:XA:186(E):C:N4  | 1:XA:191(B):G:H1   | 2.12                     | 0.43              |
| 1:XA:960:U:H4'    | 1:XA:961:U:C5'     | 2.48                     | 0.43              |
| 1:XA:1158:C:H4'   | 2:XB:133:LYS:HZ3   | 1.83                     | 0.43              |
| 2:XB:215:LEU:HA   | 2:XB:215:LEU:HD22  | 1.73                     | 0.43              |
| 1:XA:877:C:H5"    | 8:XH:88:LYS:HD3    | 2.00                     | 0.43              |
| 10:XJ:54:PHE:CZ   | 10:XJ:55:LYS:HE3   | 2.54                     | 0.43              |
| 15:XO:25:THR:HG21 | 15:XO:70:LEU:HB2   | 2.01                     | 0.43              |
| 20:XT:98:PRO:C    | 20:XT:100:ILE:H    | 2.21                     | 0.43              |
| 22:XV:28:C:H2'    | 22:XV:29:G:C8      | 2.53                     | 0.43              |
| 47:Y1:25:LYS:C    | 47:Y1:27:GLU:H     | 2.22                     | 0.43              |
| 48:Y2:15:LYS:H    | 48:Y2:67:LYS:CE    | 2.32                     | 0.43              |
| 25:YA:1173:G:H4'  | 25:YA:1174:A:N7    | 2.33                     | 0.43              |
| 25:YA:1694:C:H4'  | 25:YA:1695:G:O5'   | 2.18                     | 0.43              |
| 25:YA:651:G:OP1   | 54:Y8:19:SER:N     | 2.47                     | 0.43              |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2  | 2.54                     | 0.43              |
| 28:YE:87:GLU:O    | 28:YE:89:ASP:N     | 2.50                     | 0.43              |
| 29:YF:33:LEU:HD12 | 29:YF:33:LEU:HA    | 1.87                     | 0.43              |
| 29:YF:64:ILE:HG23 | 29:YF:65:TRP:CD1   | 2.53                     | 0.43              |
| 34:YO:88:ASN:OD1  | 34:YO:90:GLN:HB2   | 2.19                     | 0.43              |
| 35:YP:83:VAL:O    | 35:YP:114:ILE:HA   | 2.19                     | 0.43              |
| 43:YX:72:LYS:HG2  | 43:YX:73:ARG:O     | 2.18                     | 0.43              |
| 56:Z7:8:LYS:HG3   | 56:Z7:9:LYS:H      | 1.83                     | 0.43              |
| 1:QA:1299:A:C6    | 1:QA:1301:U:C2     | 3.06                     | 0.43              |
| 1:QA:452:A:O2'    | 1:QA:453:A:O5'     | 2.36                     | 0.43              |
| 1:QA:767:A:H2'    | 1:QA:768:A:O4'     | 2.18                     | 0.43              |
| 25:RA:1337:G:H2'  | 25:RA:1338:G:C8    | 2.53                     | 0.43              |
| 25:RA:134:C:H2'   | 25:RA:135:G:H8     | 1.82                     | 0.43              |
| 25:RA:2713:A:OP1  | 37:RR:14:SER:OG    | 2.30                     | 0.43              |
| 36:RQ:116:GLU:O   | 36:RQ:120:ILE:HG12 | 2.17                     | 0.43              |
| 39:RT:1:MET:O     | 39:RT:3:ARG:HG2    | 2.19                     | 0.43              |
| 44:RY:47:LYS:O    | 44:RY:49:VAL:N     | 2.51                     | 0.43              |
| 1:XA:743:U:H2'    | 1:XA:744:C:C6      | 2.54                     | 0.43              |
| 1:XA:757:U:H2'    | 1:XA:758:G:O4'     | 2.18                     | 0.43              |
| 1:XA:977:A:O2'    | 1:XA:981:U:N3      | 2.47                     | 0.43              |
| 2:XB:37:ASN:C     | 2:XB:39:ILE:H      | 2.20                     | 0.43              |
| 2:XB:80:ILE:HG21  | 2:XB:212:GLN:HA    | 2.00                     | 0.43              |
| 49:Y3:51:ALA:HA   | 49:Y3:54:VAL:HG12  | 2.00                     | 0.43              |
| 25:YA:1223:C:OP2  | 41:YV:88:ARG:NH1   | 2.51                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1530:G:O6    | 25:YA:1542:G:N2   | 2.52                     | 0.43              |
| 25:YA:1680:U:O2    | 25:YA:1763:G:H3'  | 2.18                     | 0.43              |
| 25:YA:826:U:OP1    | 25:YA:2429:G:OP1  | 2.36                     | 0.43              |
| 22:XV:76:A:O2'     | 25:YA:2451:A:O2'  | 2.19                     | 0.43              |
| 26:YB:15:A:H1'     | 26:YB:109:G:C4    | 2.53                     | 0.43              |
| 32:YI:110:ASP:HB3  | 32:YI:112:LYS:N   | 2.33                     | 0.43              |
| 33:YN:112:LEU:HG   | 33:YN:112:LEU:O   | 2.17                     | 0.43              |
| 34:YO:64:ARG:HG2   | 34:YO:79:PHE:CD1  | 2.54                     | 0.43              |
| 45:YZ:5:LEU:HB3    | 45:YZ:59:LEU:HA   | 2.00                     | 0.43              |
| 8:QH:105:ARG:HD3   | 8:QH:105:ARG:HA   | 1.78                     | 0.43              |
| 16:QP:20:VAL:HG21  | 16:QP:32:TYR:CE2  | 2.54                     | 0.43              |
| 25:RA:1638:C:H5''  | 25:RA:2710:C:O2'  | 2.19                     | 0.43              |
| 25:RA:443:A:H1'    | 25:RA:1201:C:O4'  | 2.17                     | 0.43              |
| 35:RP:90:ARG:HB3   | 35:RP:91:PHE:H    | 1.68                     | 0.43              |
| 9:XI:8:GLY:HA2     | 9:XI:79:LEU:HD12  | 2.01                     | 0.43              |
| 10:XJ:44:VAL:HG13  | 10:XJ:66:ARG:HG2  | 1.99                     | 0.43              |
| 12:XL:58:VAL:O     | 12:XL:65:GLU:HA   | 2.18                     | 0.43              |
| 13:XM:7:VAL:HA     | 50:Y4:34:GLU:OE1  | 2.19                     | 0.43              |
| 14:YN:27:CYS:SG    | 14:YN:29:ARG:HB2  | 2.58                     | 0.43              |
| 16:XP:45:THR:HG22  | 16:XP:47:ASP:N    | 2.26                     | 0.43              |
| 47:Y1:94:LEU:HD23  | 47:Y1:94:LEU:HA   | 1.82                     | 0.43              |
| 50:Y4:43:TYR:CD1   | 50:Y4:43:TYR:C    | 2.92                     | 0.43              |
| 37:YR:33:ARG:HH21  | 51:Y5:55:ARG:HG2  | 1.82                     | 0.43              |
| 53:Y7:47:ARG:HB2   | 53:Y7:48:LYS:H    | 1.59                     | 0.43              |
| 25:YA:1054:A:H5'   | 25:YA:1055:G:OP2  | 2.18                     | 0.43              |
| 25:YA:1359:A:N6    | 25:YA:1373:A:C4   | 2.87                     | 0.43              |
| 25:YA:1870:C:H2'   | 25:YA:1871:A:O4'  | 2.18                     | 0.43              |
| 25:YA:1903:G:OP2   | 27:YD:241:PRO:HB2 | 2.19                     | 0.43              |
| 25:YA:1910:G:H1    | 25:YA:1920:C:N4   | 2.15                     | 0.43              |
| 25:YA:1916:A:H2'   | 25:YA:1917:U:O4'  | 2.18                     | 0.43              |
| 25:YA:2308:G:H22   | 25:YA:2311:A:H2   | 1.66                     | 0.43              |
| 25:YA:582:G:H2'    | 25:YA:583:G:C8    | 2.54                     | 0.43              |
| 25:YA:67:U:C2      | 25:YA:74:A:H2     | 2.35                     | 0.43              |
| 27:YD:132:PRO:HG3  | 27:YD:190:TYR:CE1 | 2.54                     | 0.43              |
| 35:YP:126:VAL:HG22 | 35:YP:145:PRO:HG2 | 2.00                     | 0.43              |
| 44:YY:67:LEU:HA    | 44:YY:67:LEU:HD12 | 1.78                     | 0.43              |
| 44:YY:80:GLY:O     | 44:YY:81:LYS:HG3  | 2.18                     | 0.43              |
| 45:YZ:52:SER:OG    | 45:YZ:52:SER:O    | 2.30                     | 0.43              |
| 1:QA:1321:C:H4'    | 13:QM:87:TYR:CZ   | 2.54                     | 0.43              |
| 1:QA:1511:G:H2'    | 1:QA:1512:U:O4'   | 2.19                     | 0.43              |
| 1:QA:157:G:H1      | 1:QA:164:U:H3     | 1.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:842:C:O2'     | 1:QA:848:C:N4      | 2.51                     | 0.43              |
| 1:QA:857:C:H2'     | 1:QA:858:G:O4'     | 2.19                     | 0.43              |
| 4:QD:133:VAL:HG12  | 4:QD:135:LEU:H     | 1.83                     | 0.43              |
| 8:QH:13:ILE:O      | 8:QH:17:THR:HG23   | 2.19                     | 0.43              |
| 9:QI:112:LYS:HD3   | 9:QI:113:LYS:O     | 2.18                     | 0.43              |
| 14:QN:47:LEU:HA    | 14:QN:47:LEU:HD23  | 1.74                     | 0.43              |
| 6:QF:99:ALA:HB1    | 18:QR:23:LYS:HZ2   | 1.83                     | 0.43              |
| 54:R8:58:ILE:HA    | 54:R8:61:LEU:HD21  | 2.01                     | 0.43              |
| 25:RA:1101:U:H2'   | 25:RA:1102:C:H6    | 1.83                     | 0.43              |
| 25:RA:1291:C:H2'   | 25:RA:1292:U:C6    | 2.52                     | 0.43              |
| 25:RA:1728:G:H5'   | 25:RA:1729:A:OP2   | 2.18                     | 0.43              |
| 25:RA:1780:A:O2'   | 25:RA:1781:C:O2    | 2.31                     | 0.43              |
| 25:RA:2170:A:H2'   | 25:RA:2171:A:O4'   | 2.18                     | 0.43              |
| 25:RA:519:U:H2'    | 25:RA:520:G:C8     | 2.54                     | 0.43              |
| 28:RE:14:ILE:H     | 28:RE:21:VAL:HA    | 1.84                     | 0.43              |
| 28:RE:179:GLU:HB3  | 28:RE:181:LEU:HD22 | 1.99                     | 0.43              |
| 35:RP:65:ARG:O     | 35:RP:68:GLN:NE2   | 2.50                     | 0.43              |
| 38:RS:88:ASP:CG    | 38:RS:89:ARG:H     | 2.21                     | 0.43              |
| 42:RW:20:VAL:HG22  | 42:RW:47:VAL:HG21  | 2.00                     | 0.43              |
| 44:RY:55:TYR:N     | 44:RY:55:TYR:CD1   | 2.87                     | 0.43              |
| 44:RY:46:LYS:HB2   | 44:RY:61:ILE:HG22  | 1.99                     | 0.43              |
| 1:XA:22:G:H2'      | 1:XA:23:C:C6       | 2.53                     | 0.43              |
| 2:XB:100:GLY:N     | 2:XB:176:GLU:OE2   | 2.47                     | 0.43              |
| 4:XD:196:LEU:O     | 4:XD:198:VAL:N     | 2.51                     | 0.43              |
| 17:XQ:62:SER:HB3   | 17:XQ:72:ARG:HE    | 1.84                     | 0.43              |
| 22:XV:2:C:C2'      | 22:XV:3:G:H5'      | 2.48                     | 0.43              |
| 50:Y4:55:ARG:C     | 50:Y4:59:PHE:HB3   | 2.39                     | 0.43              |
| 25:YA:1952:A:C5    | 34:YO:22:ILE:HD12  | 2.54                     | 0.43              |
| 25:YA:226:G:H2'    | 25:YA:227:A:C8     | 2.54                     | 0.43              |
| 25:YA:2615:U:C2    | 51:Y5:7:PRO:HA     | 2.52                     | 0.43              |
| 25:YA:265:A:O2'    | 25:YA:266:G:H4'    | 2.18                     | 0.43              |
| 25:YA:363(A):A:H2' | 25:YA:363(B):G:C8  | 2.54                     | 0.43              |
| 25:YA:273(C):C:N4  | 25:YA:363(C):G:H1  | 2.15                     | 0.43              |
| 28:YE:119:ARG:HG2  | 28:YE:160:TYR:HB2  | 2.00                     | 0.43              |
| 28:YE:14:ILE:HG23  | 28:YE:15:PHE:N     | 2.34                     | 0.43              |
| 31:YH:152:ARG:O    | 31:YH:153:LYS:HB2  | 2.19                     | 0.43              |
| 38:YS:39:ILE:HD12  | 38:YS:85:VAL:HG11  | 2.00                     | 0.43              |
| 41:YV:55:ALA:HB2   | 41:YV:101:GLY:HA2  | 2.00                     | 0.43              |
| 45:YZ:52:SER:C     | 45:YZ:54:HIS:H     | 2.22                     | 0.43              |
| 1:QA:601:C:H2'     | 1:QA:602:A:H8      | 1.83                     | 0.43              |
| 2:QB:8:LYS:HE3     | 2:QB:11:LEU:HB3    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:QB:167:PRO:HG3  | 2:QB:188:ALA:HB2  | 2.01                     | 0.43              |
| 12:QL:85:ILE:HD12 | 12:QL:85:ILE:HA   | 1.75                     | 0.43              |
| 13:QM:44:ARG:HB2  | 13:QM:47:ASP:OD2  | 2.19                     | 0.43              |
| 17:QQ:45:HIS:NE2  | 17:QQ:47:PRO:HG3  | 2.34                     | 0.43              |
| 23:QW:16:U:H5'    | 23:QW:17:C:OP2    | 2.18                     | 0.43              |
| 25:RA:1308:A:H2'  | 25:RA:1309:G:O4'  | 2.17                     | 0.43              |
| 25:RA:2133:G:O2'  | 25:RA:2158:A:N1   | 2.52                     | 0.43              |
| 25:RA:2376:A:H2'  | 25:RA:2377:A:O4'  | 2.18                     | 0.43              |
| 25:RA:631:A:H2'   | 25:RA:632:A:O4'   | 2.18                     | 0.43              |
| 25:RA:671:C:H2'   | 25:RA:672:C:C6    | 2.54                     | 0.43              |
| 27:RD:35:LYS:HE3  | 27:RD:64:ILE:C    | 2.39                     | 0.43              |
| 29:RF:9:ILE:HG23  | 29:RF:20:LEU:O    | 2.18                     | 0.43              |
| 35:RP:18:ARG:HD2  | 35:RP:27:HIS:CD2  | 2.54                     | 0.43              |
| 36:RQ:20:ALA:HA   | 36:RQ:98:LYS:HB3  | 2.00                     | 0.43              |
| 39:RT:19:LEU:HA   | 39:RT:20:PRO:HD3  | 1.86                     | 0.43              |
| 1:XA:1005:A:HO2'  | 1:XA:1037:C:HO2'  | 1.62                     | 0.43              |
| 1:XA:1298:C:H4'   | 1:XA:1299:A:N9    | 2.34                     | 0.43              |
| 1:XA:1301:U:H2'   | 1:XA:1301:U:O2    | 2.18                     | 0.43              |
| 1:XA:134:A:H61    | 16:XP:25:ARG:NH1  | 2.17                     | 0.43              |
| 1:XA:1392:G:H2'   | 1:XA:1393:U:C6    | 2.53                     | 0.43              |
| 1:XA:1436:U:H2'   | 1:XA:1437:C:O4'   | 2.18                     | 0.43              |
| 1:XA:603:U:H2'    | 1:XA:604:G:C8     | 2.54                     | 0.43              |
| 1:XA:636:U:H2'    | 1:XA:637:G:C8     | 2.54                     | 0.43              |
| 1:XA:672:U:H2'    | 1:XA:673:G:C8     | 2.54                     | 0.43              |
| 2:XB:212:GLN:NE2  | 2:XB:216:SER:HB2  | 2.34                     | 0.43              |
| 2:XB:7:VAL:HG21   | 2:XB:217:ARG:NH1  | 2.34                     | 0.43              |
| 5:XE:42:GLY:CA    | 5:XE:66:MET:HG2   | 2.48                     | 0.43              |
| 5:XE:69:VAL:O     | 5:XE:71:LEU:N     | 2.51                     | 0.43              |
| 7:XG:140:ASP:HA   | 7:XG:143:ARG:NH1  | 2.34                     | 0.43              |
| 1:XA:1373:G:O3'   | 7:XG:36:LYS:NZ    | 2.51                     | 0.43              |
| 12:XL:110:VAL:CG2 | 12:XL:120:TYR:HB3 | 2.48                     | 0.43              |
| 12:XL:59:ARG:NH1  | 12:XL:65:GLU:OE2  | 2.51                     | 0.43              |
| 14:XN:6:LEU:HD23  | 14:XN:23:ARG:HH22 | 1.83                     | 0.43              |
| 26:YB:12:C:O2'    | 46:Y0:74:ARG:HG3  | 2.19                     | 0.43              |
| 50:Y4:6:HIS:HA    | 50:Y4:7:PRO:HD2   | 1.82                     | 0.43              |
| 25:YA:1231:G:H2'  | 25:YA:1232:G:C8   | 2.54                     | 0.43              |
| 25:YA:1607:C:H5'' | 25:YA:1608:A:H5'  | 2.01                     | 0.43              |
| 25:YA:1799:G:H4'  | 25:YA:1800:C:O5'  | 2.18                     | 0.43              |
| 25:YA:2780:G:P    | 33:YN:118:LYS:HE2 | 2.58                     | 0.43              |
| 28:YE:4:ILE:HD12  | 28:YE:28:ALA:HB1  | 2.01                     | 0.43              |
| 30:YG:145:THR:O   | 30:YG:147:ASP:N   | 2.44                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:YG:31:VAL:HA     | 30:YG:32:PRO:HD3   | 1.83                     | 0.43              |
| 35:YP:15:ARG:O      | 35:YP:17:LYS:HG3   | 2.19                     | 0.43              |
| 35:YP:30:THR:O      | 35:YP:33:ARG:HB2   | 2.18                     | 0.43              |
| 25:YA:1190:G:H5'    | 35:YP:32:THR:HA    | 2.01                     | 0.43              |
| 35:YP:5:ASP:O       | 35:YP:6:LEU:C      | 2.57                     | 0.43              |
| 44:YY:87:LYS:HB2    | 44:YY:87:LYS:NZ    | 2.34                     | 0.43              |
| 1:QA:1179:A:H2'     | 1:QA:1180:A:O4'    | 2.19                     | 0.43              |
| 1:QA:1488:G:H2'     | 1:QA:1489:G:C8     | 2.53                     | 0.43              |
| 1:QA:24:U:H2'       | 1:QA:25:C:H6       | 1.84                     | 0.43              |
| 1:QA:266:G:O2'      | 1:QA:267:C:OP2     | 2.32                     | 0.43              |
| 1:QA:383:A:O5'      | 1:QA:383:A:H8      | 2.02                     | 0.43              |
| 4:QD:155:LEU:O      | 4:QD:159:ARG:HG2   | 2.19                     | 0.43              |
| 5:QE:18:ARG:HE      | 5:QE:18:ARG:HB3    | 1.52                     | 0.43              |
| 1:QA:1346:A:H2'     | 7:QG:10:ARG:HH22   | 1.83                     | 0.43              |
| 8:QH:101:PRO:HG2    | 8:QH:133:LEU:HD11  | 2.01                     | 0.43              |
| 9:QI:17:VAL:HG11    | 9:QI:81:ILE:HD13   | 2.00                     | 0.43              |
| 25:RA:242:G:H3'     | 54:R8:6:THR:HG23   | 2.01                     | 0.43              |
| 25:RA:1245:G:OP1    | 35:RP:13:ASN:ND2   | 2.50                     | 0.43              |
| 25:RA:1444(A):A:H4' | 25:RA:1460:A:O2'   | 2.18                     | 0.43              |
| 25:RA:1492:G:H3'    | 25:RA:1493:C:H5'   | 2.01                     | 0.43              |
| 25:RA:2058:A:H8     | 25:RA:2058:A:O5'   | 2.02                     | 0.43              |
| 25:RA:2336:A:H61    | 46:R0:43:THR:CG2   | 2.32                     | 0.43              |
| 25:RA:2517:C:C2     | 25:RA:2542:A:N6    | 2.87                     | 0.43              |
| 25:RA:2563:U:H2'    | 25:RA:2565:A:OP2   | 2.19                     | 0.43              |
| 28:RE:34:VAL:HG23   | 28:RE:64:LYS:HZ2   | 1.84                     | 0.43              |
| 25:RA:2749:A:H4'    | 31:RH:62:LYS:HB3   | 2.01                     | 0.43              |
| 32:RI:68:LEU:HA     | 32:RI:71:ILE:HG22  | 2.00                     | 0.43              |
| 36:RQ:104:PHE:CE2   | 36:RQ:125:LEU:HD11 | 2.53                     | 0.43              |
| 39:RT:107:ASP:O     | 39:RT:110:ILE:HG22 | 2.19                     | 0.43              |
| 2:XB:172:ILE:O      | 2:XB:175:ARG:HB3   | 2.18                     | 0.43              |
| 3:XC:149:ALA:HA     | 3:XC:201:TYR:O     | 2.18                     | 0.43              |
| 5:XE:9:LYS:HE3      | 5:XE:9:LYS:HB2     | 1.89                     | 0.43              |
| 6:XF:30:LEU:HB3     | 6:XF:35:ALA:HB3    | 2.01                     | 0.43              |
| 13:XM:4:ILE:HG22    | 13:XM:5:ALA:N      | 2.34                     | 0.43              |
| 19:XS:68:GLY:HA3    | 50:Y4:59:PHE:CE1   | 2.43                     | 0.43              |
| 23:XW:60:U:O2'      | 23:XW:61:C:H5'     | 2.19                     | 0.43              |
| 25:YA:857:C:H1'     | 46:Y0:26:TYR:CE1   | 2.54                     | 0.43              |
| 48:Y2:17:SER:HB3    | 48:Y2:67:LYS:HE3   | 2.00                     | 0.43              |
| 48:Y2:61:LEU:HD23   | 48:Y2:61:LEU:HA    | 1.85                     | 0.43              |
| 52:Y6:28:ARG:HH21   | 52:Y6:30:THR:HG23  | 1.84                     | 0.43              |
| 25:YA:2371:G:O2'    | 52:Y6:45:LYS:HB3   | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:118:A:N3     | 25:YA:178:G:H1'    | 2.34                     | 0.43              |
| 25:YA:579:G:O2'    | 25:YA:2019:A:OP1   | 2.29                     | 0.43              |
| 25:YA:242:G:H1'    | 25:YA:243:U:OP2    | 2.18                     | 0.43              |
| 25:YA:746:A:C6     | 25:YA:2611:U:H5''  | 2.54                     | 0.43              |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:C8  | 2.54                     | 0.43              |
| 25:YA:507:A:H5''   | 25:YA:508:G:H5'    | 2.01                     | 0.43              |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:H    | 1.83                     | 0.43              |
| 30:YG:103:LEU:HA   | 30:YG:103:LEU:HD23 | 1.83                     | 0.43              |
| 35:YP:113:LYS:HG2  | 35:YP:115:LEU:HD23 | 2.01                     | 0.43              |
| 39:YT:80:SER:HA    | 39:YT:81:PRO:HD3   | 1.89                     | 0.43              |
| 43:YX:53:LYS:H     | 43:YX:82:GLN:HB3   | 1.83                     | 0.43              |
| 1:QA:999:U:H2'     | 1:QA:1000:A:C8     | 2.54                     | 0.43              |
| 1:QA:398:C:H2'     | 1:QA:399:G:H8      | 1.84                     | 0.43              |
| 1:QA:579:G:H2'     | 1:QA:580:U:C6      | 2.54                     | 0.43              |
| 3:QC:11:ARG:HB3    | 3:QC:15:THR:HB     | 2.01                     | 0.43              |
| 13:QM:3:ARG:NH2    | 30:RG:139:LEU:HD13 | 2.34                     | 0.43              |
| 52:R6:7:ILE:HG13   | 52:R6:8:LYS:H      | 1.84                     | 0.43              |
| 25:RA:2059:A:H5'   | 25:RA:2060:A:OP2   | 2.19                     | 0.43              |
| 25:RA:2849:U:O4    | 39:RT:23:ARG:NH2   | 2.40                     | 0.43              |
| 25:RA:395:U:H2'    | 25:RA:396:G:C8     | 2.53                     | 0.43              |
| 28:RE:116:VAL:HG11 | 28:RE:138:PRO:HB3  | 2.01                     | 0.43              |
| 28:RE:48:GLN:OE1   | 28:RE:64:LYS:NZ    | 2.52                     | 0.43              |
| 29:RF:34:TRP:CE3   | 29:RF:35:GLU:HG2   | 2.54                     | 0.43              |
| 31:RH:124:GLU:HB3  | 31:RH:132:ARG:CG   | 2.48                     | 0.43              |
| 32:RI:31:LEU:HD11  | 32:RI:38:LEU:HG    | 2.00                     | 0.43              |
| 36:RQ:81:VAL:C     | 36:RQ:82:ARG:CG    | 2.85                     | 0.43              |
| 38:RS:12:PHE:HD1   | 38:RS:12:PHE:HA    | 1.72                     | 0.43              |
| 34:RO:104:ARG:HD3  | 39:RT:36:GLU:OE2   | 2.19                     | 0.43              |
| 25:RA:2684:U:OP1   | 39:RT:53:ARG:HD3   | 2.19                     | 0.43              |
| 44:RY:54:LYS:HB3   | 44:RY:55:TYR:CD1   | 2.53                     | 0.43              |
| 45:RZ:48:PHE:CE1   | 45:RZ:52:SER:HA    | 2.54                     | 0.43              |
| 1:XA:1429:C:H2'    | 1:XA:1430:C:H6     | 1.83                     | 0.43              |
| 1:XA:1494:G:N7     | 58:XA:1672:PAR:N32 | 2.66                     | 0.43              |
| 6:XF:16:GLN:HA     | 6:XF:19:LEU:CB     | 2.49                     | 0.43              |
| 8:XH:13:ILE:O      | 8:XH:17:THR:HG23   | 2.19                     | 0.43              |
| 1:XA:1316:G:H4'    | 14:XN:18:VAL:HG11  | 2.00                     | 0.43              |
| 18:XR:56:THR:HB    | 18:XR:58:LEU:HD12  | 2.01                     | 0.43              |
| 23:XW:72:C:H2'     | 23:XW:73:A:O4'     | 2.19                     | 0.43              |
| 47:Y1:58:ILE:HG23  | 47:Y1:87:PRO:HG3   | 2.01                     | 0.43              |
| 49:Y3:7:LYS:HE2    | 49:Y3:32:GLN:O     | 2.19                     | 0.43              |
| 50:Y4:14:ILE:HG13  | 50:Y4:31:ILE:HB    | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Y6:41:PRO:HG2   | 52:Y6:45:LYS:N     | 2.29                     | 0.43              |
| 25:YA:1373:A:C6    | 25:YA:1374:G:C4    | 3.07                     | 0.43              |
| 25:YA:1952:A:N3    | 25:YA:2560:C:O2'   | 2.49                     | 0.43              |
| 25:YA:630:G:N2     | 25:YA:633:A:OP2    | 2.45                     | 0.43              |
| 27:YD:134:ARG:HD3  | 27:YD:135:PHE:CE1  | 2.54                     | 0.43              |
| 28:YE:111:ARG:HD2  | 28:YE:160:TYR:CE2  | 2.54                     | 0.43              |
| 28:YE:36:ARG:HH21  | 28:YE:88:GLY:CA    | 2.32                     | 0.43              |
| 36:YQ:45:GLN:H     | 36:YQ:45:GLN:CD    | 2.22                     | 0.43              |
| 38:YS:30:ARG:NH2   | 38:YS:92:TYR:CD1   | 2.87                     | 0.43              |
| 25:YA:751:A:H5'    | 42:YW:90:ARG:HA    | 1.99                     | 0.43              |
| 25:YA:1342:A:OP1   | 43:YX:36:LYS:NZ    | 2.52                     | 0.43              |
| 25:YA:897:C:H4'    | 45:YZ:182:LYS:HD2  | 2.01                     | 0.43              |
| 1:QA:384:G:H2'     | 1:QA:385:C:C6      | 2.54                     | 0.42              |
| 1:QA:580:U:H2'     | 1:QA:581:G:O4'     | 2.18                     | 0.42              |
| 1:QA:612:C:O2      | 1:QA:629:G:N2      | 2.52                     | 0.42              |
| 1:QA:901:A:H8      | 1:QA:901:A:O5'     | 2.02                     | 0.42              |
| 4:QD:158:ILE:HA    | 4:QD:158:ILE:HD13  | 1.82                     | 0.42              |
| 6:QF:62:TRP:CH2    | 6:QF:64:GLN:HB2    | 2.54                     | 0.42              |
| 7:QG:102:ARG:HG2   | 7:QG:106:GLN:OE1   | 2.19                     | 0.42              |
| 8:QH:25:ASP:OD1    | 8:QH:25:ASP:N      | 2.50                     | 0.42              |
| 13:QM:4:ILE:H      | 13:QM:9:ILE:HG22   | 1.84                     | 0.42              |
| 18:QR:53:ARG:HH21  | 18:QR:60:ALA:N     | 2.17                     | 0.42              |
| 23:QW:37:A:H2'     | 23:QW:38:A:O4'     | 2.19                     | 0.42              |
| 46:R0:51:VAL:N     | 46:R0:62:LEU:HD12  | 2.33                     | 0.42              |
| 52:R6:17:LYS:HB3   | 52:R6:44:ARG:NH2   | 2.30                     | 0.42              |
| 52:R6:8:LYS:O      | 52:R6:27:LYS:HA    | 2.18                     | 0.42              |
| 25:RA:1005:C:O2'   | 33:RN:28:THR:HG21  | 2.18                     | 0.42              |
| 25:RA:1022:G:H22   | 25:RA:1142(A):A:H2 | 1.66                     | 0.42              |
| 25:RA:1543:A:HO2'  | 25:RA:1544:C:H3'   | 1.82                     | 0.42              |
| 25:RA:2626:C:H2'   | 25:RA:2627:G:O4'   | 2.19                     | 0.42              |
| 25:RA:2869:G:H2'   | 25:RA:2870:C:O4'   | 2.18                     | 0.42              |
| 27:RD:169:GLU:N    | 27:RD:172:TYR:O    | 2.52                     | 0.42              |
| 28:RE:117:MET:HB2  | 28:RE:122:PHE:O    | 2.18                     | 0.42              |
| 33:RN:61:ARG:HA    | 33:RN:61:ARG:HE    | 1.82                     | 0.42              |
| 40:RU:69:CYS:HB3   | 40:RU:106:PHE:CZ   | 2.54                     | 0.42              |
| 41:RV:64:HIS:CG    | 41:RV:92:THR:HG22  | 2.52                     | 0.42              |
| 45:RZ:111:VAL:HG13 | 45:RZ:112:ARG:H    | 1.83                     | 0.42              |
| 45:RZ:115:GLY:HA2  | 45:RZ:175:VAL:O    | 2.19                     | 0.42              |
| 1:XA:1490:C:H2'    | 1:XA:1491:G:H8     | 1.84                     | 0.42              |
| 1:XA:377:G:OP1     | 16:XP:5:ARG:NH1    | 2.47                     | 0.42              |
| 1:XA:755:G:OP2     | 15:XO:65:ARG:HG2   | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:38:LEU:O      | 7:XG:38:LEU:HD12   | 2.20                     | 0.42              |
| 25:YA:1291:C:H2'   | 25:YA:1292:U:C6    | 2.54                     | 0.42              |
| 25:YA:1794:U:H2'   | 25:YA:1795:C:C6    | 2.53                     | 0.42              |
| 25:YA:2364:C:H2'   | 25:YA:2365:G:O4'   | 2.18                     | 0.42              |
| 25:YA:2564:A:C2    | 25:YA:2647:U:H4'   | 2.53                     | 0.42              |
| 25:YA:277:C:H3'    | 25:YA:278:A:C5'    | 2.49                     | 0.42              |
| 25:YA:2783:G:H2'   | 25:YA:2784:C:C6    | 2.54                     | 0.42              |
| 25:YA:443:A:H1'    | 25:YA:1201:C:O4'   | 2.19                     | 0.42              |
| 25:YA:512:G:OP1    | 25:YA:1234:U:O2'   | 2.33                     | 0.42              |
| 26:YB:81:G:O6      | 26:YB:95:U:C2      | 2.72                     | 0.42              |
| 27:YD:248:SER:HB3  | 27:YD:252:TRP:CD2  | 2.54                     | 0.42              |
| 25:YA:1354:A:OP1   | 27:YD:38:LYS:HE2   | 2.18                     | 0.42              |
| 31:YH:126:PRO:HB2  | 31:YH:127:GLU:H    | 1.59                     | 0.42              |
| 33:YN:134:ARG:H    | 33:YN:135:PRO:HD3  | 1.83                     | 0.42              |
| 34:YO:88:ASN:ND2   | 34:YO:92:GLU:HB2   | 2.23                     | 0.42              |
| 41:YV:64:HIS:ND1   | 41:YV:92:THR:HG22  | 2.34                     | 0.42              |
| 1:QA:1192:C:O2     | 5:QE:25:ARG:NH2    | 2.50                     | 0.42              |
| 1:QA:701:C:H1'     | 1:QA:703:G:C6      | 2.54                     | 0.42              |
| 1:QA:986:A:N3      | 19:QS:52:TYR:OH    | 2.46                     | 0.42              |
| 4:QD:108:LEU:HD21  | 4:QD:183:GLY:HA3   | 2.01                     | 0.42              |
| 9:QI:48:GLU:N      | 9:QI:49:PRO:HD2    | 2.34                     | 0.42              |
| 15:QO:25:THR:HG21  | 15:QO:70:LEU:HB2   | 2.00                     | 0.42              |
| 18:QR:29:PHE:N     | 18:QR:29:PHE:CD1   | 2.87                     | 0.42              |
| 19:QS:41:VAL:HG12  | 19:QS:44:MET:HB2   | 2.02                     | 0.42              |
| 25:RA:1126:A:OP1   | 25:RA:1126:A:H8    | 2.03                     | 0.42              |
| 25:RA:1756:G:H4'   | 25:RA:1758:G:O4'   | 2.19                     | 0.42              |
| 25:RA:2695:C:H2'   | 25:RA:2696:U:H6    | 1.84                     | 0.42              |
| 25:RA:622:G:H2'    | 25:RA:623:G:C8     | 2.54                     | 0.42              |
| 28:RE:22:PRO:O     | 28:RE:22:PRO:HD2   | 2.19                     | 0.42              |
| 31:RH:153:LYS:HD2  | 31:RH:153:LYS:N    | 2.33                     | 0.42              |
| 33:RN:96:GLU:HB2   | 33:RN:122:VAL:HG12 | 2.00                     | 0.42              |
| 33:RN:89:LYS:O     | 33:RN:93:THR:HG22  | 2.19                     | 0.42              |
| 35:RP:100:LEU:HD22 | 35:RP:100:LEU:HA   | 1.77                     | 0.42              |
| 25:RA:2319:G:O6    | 38:RS:4:LEU:HB2    | 2.19                     | 0.42              |
| 25:RA:994:C:OP1    | 40:RU:53:ARG:NH2   | 2.52                     | 0.42              |
| 45:RZ:69:THR:HG22  | 45:RZ:90:VAL:HA    | 1.99                     | 0.42              |
| 1:XA:1352:C:N4     | 1:XA:1370:G:H1     | 2.13                     | 0.42              |
| 1:XA:19:C:OP1      | 5:XE:125:SER:OG    | 2.29                     | 0.42              |
| 1:XA:397:A:H5'     | 1:XA:398:C:OP1     | 2.19                     | 0.42              |
| 1:XA:769:G:H4'     | 1:XA:1513:A:H4'    | 2.00                     | 0.42              |
| 2:XB:68:ILE:HB     | 2:XB:70:PHE:HE1    | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:XF:100:ASN:ND2   | 18:XR:26:LEU:O     | 2.51                     | 0.42              |
| 10:XJ:6:ILE:HG22   | 10:XJ:98:ILE:HG23  | 2.02                     | 0.42              |
| 12:XL:28:LYS:HB3   | 12:XL:30:ALA:HB2   | 2.01                     | 0.42              |
| 25:YA:2336:A:H61   | 46:Y0:43:THR:HG21  | 1.84                     | 0.42              |
| 48:Y2:8:LYS:HB2    | 48:Y2:8:LYS:HE3    | 1.83                     | 0.42              |
| 25:YA:1063:G:H22   | 25:YA:1076:C:H1'   | 1.84                     | 0.42              |
| 25:YA:2448:A:OP2   | 25:YA:2499:C:OP2   | 2.36                     | 0.42              |
| 25:YA:278:A:H4'    | 25:YA:279:C:OP1    | 2.19                     | 0.42              |
| 25:YA:323:G:H1'    | 25:YA:1205:U:O2    | 2.19                     | 0.42              |
| 25:YA:372:G:O2'    | 25:YA:373:U:P      | 2.77                     | 0.42              |
| 25:YA:845:G:OP2    | 25:YA:845:G:H8     | 2.02                     | 0.42              |
| 35:YP:125:VAL:CG1  | 35:YP:138:LEU:HD21 | 2.49                     | 0.42              |
| 45:YZ:8:TYR:HA     | 45:YZ:62:PRO:HD3   | 2.00                     | 0.42              |
| 1:QA:1367:C:H5'    | 10:QJ:60:ARG:NH2   | 2.35                     | 0.42              |
| 1:QA:1499:A:H1'    | 1:QA:1520:G:H5'    | 2.01                     | 0.42              |
| 1:QA:24:U:H2'      | 1:QA:25:C:C6       | 2.54                     | 0.42              |
| 1:QA:296:U:H2'     | 1:QA:297:G:C8      | 2.54                     | 0.42              |
| 2:QB:130:ARG:HA    | 2:QB:131:PRO:HD3   | 1.81                     | 0.42              |
| 1:QA:542:G:H5'     | 4:QD:41:GLY:HA3    | 2.00                     | 0.42              |
| 11:QK:120:ARG:HA   | 11:QK:121:PRO:HD3  | 1.87                     | 0.42              |
| 7:QG:153:HIS:HB3   | 11:QK:58:PRO:HG2   | 2.01                     | 0.42              |
| 17:QQ:29:HIS:CG    | 17:QQ:30:PRO:HD2   | 2.54                     | 0.42              |
| 1:QA:1226:C:H4'    | 19:QS:80:TYR:OH    | 2.20                     | 0.42              |
| 25:RA:1184:G:OP1   | 49:R3:29:ARG:NH1   | 2.51                     | 0.42              |
| 25:RA:1188:U:H4'   | 41:RV:79:VAL:HG22  | 2.00                     | 0.42              |
| 25:RA:1508:A:O2'   | 25:RA:1509:C:O4'   | 2.36                     | 0.42              |
| 25:RA:177:G:H3'    | 25:RA:178:G:C8     | 2.52                     | 0.42              |
| 25:RA:2017:U:O2    | 51:R5:10:LYS:HB2   | 2.19                     | 0.42              |
| 26:RB:37:C:N3      | 26:RB:48:A:O2'     | 2.47                     | 0.42              |
| 27:RD:123:ALA:HA   | 27:RD:124:PRO:HD2  | 1.77                     | 0.42              |
| 25:RA:2679:A:H4'   | 28:RE:165:VAL:HG11 | 2.01                     | 0.42              |
| 32:RI:52:ARG:CB    | 32:RI:56:LYS:CB    | 2.88                     | 0.42              |
| 32:RI:88:ILE:HG12  | 32:RI:88:ILE:H     | 1.65                     | 0.42              |
| 37:RR:113:LEU:HD12 | 37:RR:113:LEU:HA   | 1.88                     | 0.42              |
| 25:RA:2820:A:C6    | 37:RR:4:LEU:HD11   | 2.54                     | 0.42              |
| 38:RS:93:LYS:HB2   | 38:RS:93:LYS:HE3   | 1.65                     | 0.42              |
| 40:RU:83:LEU:HD12  | 40:RU:113:ALA:HB2  | 2.01                     | 0.42              |
| 6:XF:95:GLU:HA     | 6:XF:96:PRO:HD3    | 1.87                     | 0.42              |
| 8:XH:104:ARG:HD2   | 8:XH:138:TRP:CD2   | 2.53                     | 0.42              |
| 9:XI:91:ASP:C      | 9:XI:93:ARG:H      | 2.21                     | 0.42              |
| 49:Y3:4:LEU:HD22   | 49:Y3:56:VAL:HG12  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:Y7:25:PRO:HA    | 53:Y7:28:ARG:CZ   | 2.49                     | 0.42              |
| 25:YA:71:A:H62     | 25:YA:114:U:H1'   | 1.84                     | 0.42              |
| 25:YA:2392:A:H2    | 25:YA:2424:C:H42  | 1.68                     | 0.42              |
| 25:YA:2629:A:O2'   | 25:YA:2630:G:H5'' | 2.19                     | 0.42              |
| 25:YA:305:U:H2'    | 25:YA:306:U:C6    | 2.54                     | 0.42              |
| 25:YA:391:G:O2'    | 25:YA:410:G:OP1   | 2.30                     | 0.42              |
| 25:YA:740:U:H2'    | 25:YA:741:G:H8    | 1.84                     | 0.42              |
| 25:YA:1567:A:H5'   | 27:YD:58:HIS:CG   | 2.54                     | 0.42              |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:N   | 2.34                     | 0.42              |
| 30:YG:64:THR:CG2   | 30:YG:66:GLN:H    | 2.28                     | 0.42              |
| 31:YH:126:PRO:HG2  | 31:YH:128:PRO:HA  | 2.00                     | 0.42              |
| 33:YN:96:GLU:HG2   | 33:YN:97:ARG:H    | 1.84                     | 0.42              |
| 35:YP:39:LYS:HG3   | 35:YP:45:LEU:CD2  | 2.45                     | 0.42              |
| 39:YT:45:PHE:CE1   | 39:YT:65:LYS:HE3  | 2.55                     | 0.42              |
| 39:YT:58:ASN:C     | 39:YT:58:ASN:HD22 | 2.23                     | 0.42              |
| 45:YZ:6:LYS:HB2    | 45:YZ:6:LYS:HE3   | 1.88                     | 0.42              |
| 1:QA:1306:A:H1'    | 1:QA:1332:A:C2    | 2.55                     | 0.42              |
| 1:QA:812:C:H1'     | 1:QA:813:U:OP2    | 2.19                     | 0.42              |
| 2:QB:217:ARG:HE    | 2:QB:217:ARG:HB2  | 1.29                     | 0.42              |
| 2:QB:21:ARG:HG3    | 2:QB:38:GLY:O     | 2.19                     | 0.42              |
| 2:QB:44:LEU:HD12   | 2:QB:44:LEU:H     | 1.83                     | 0.42              |
| 3:QC:148:GLY:HA3   | 3:QC:172:ARG:O    | 2.18                     | 0.42              |
| 3:QC:59:ARG:HH12   | 3:QC:97:LYS:HE3   | 1.84                     | 0.42              |
| 4:QD:120:LEU:HD23  | 4:QD:120:LEU:HA   | 1.86                     | 0.42              |
| 4:QD:165:MET:O     | 4:QD:166:LYS:C    | 2.54                     | 0.42              |
| 4:QD:29:PRO:C      | 4:QD:30:LYS:HD3   | 2.39                     | 0.42              |
| 4:QD:11:LEU:HD22   | 4:QD:66:ARG:HD3   | 2.02                     | 0.42              |
| 6:QF:15:ASP:OD2    | 6:QF:18:GLN:CG    | 2.66                     | 0.42              |
| 10:QJ:54:PHE:HB3   | 10:QJ:55:LYS:H    | 1.69                     | 0.42              |
| 10:QJ:79:ARG:HA    | 10:QJ:79:ARG:HD3  | 1.78                     | 0.42              |
| 14:QN:41:ARG:NH2   | 14:QN:42:ILE:HD11 | 2.35                     | 0.42              |
| 19:QS:10:PHE:CG    | 19:QS:11:VAL:N    | 2.88                     | 0.42              |
| 23:QW:67:C:H2'     | 23:QW:68:C:C6     | 2.54                     | 0.42              |
| 25:RA:459:U:H4'    | 53:R7:40:TRP:CZ3  | 2.55                     | 0.42              |
| 25:RA:1543:A:H2    | 25:RA:1545:A:C8   | 2.35                     | 0.42              |
| 25:RA:1819:A:H4'   | 25:RA:1820:U:O5'  | 2.18                     | 0.42              |
| 25:RA:2119:A:C2    | 25:RA:2171:A:H1'  | 2.55                     | 0.42              |
| 25:RA:2630:G:H2'   | 25:RA:2631:G:C8   | 2.55                     | 0.42              |
| 25:RA:2633:G:H2'   | 25:RA:2634:G:O4'  | 2.18                     | 0.42              |
| 25:RA:2723:C:OP2   | 28:RE:109:LYS:NZ  | 2.52                     | 0.42              |
| 25:RA:464:U:H2'    | 25:RA:465:G:O4'   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:987:G:H2'   | 25:RA:988:A:O4'    | 2.20                     | 0.42              |
| 27:RD:33:LEU:HB3  | 27:RD:34:VAL:H     | 1.64                     | 0.42              |
| 28:RE:9:VAL:HG23  | 28:RE:26:ILE:HA    | 2.00                     | 0.42              |
| 29:RF:78:ILE:HG13 | 29:RF:78:ILE:H     | 1.66                     | 0.42              |
| 31:RH:16:SER:OG   | 31:RH:26:VAL:O     | 2.30                     | 0.42              |
| 33:RN:30:ILE:HG23 | 33:RN:52:VAL:HG11  | 1.99                     | 0.42              |
| 38:RS:39:ILE:HD11 | 38:RS:73:LEU:HD11  | 2.00                     | 0.42              |
| 25:RA:581:C:OP1   | 40:RU:33:ARG:HG3   | 2.20                     | 0.42              |
| 45:RZ:181:GLU:HB3 | 45:RZ:182:LYS:H    | 1.61                     | 0.42              |
| 1:XA:258:G:H2'    | 1:XA:259:G:H8      | 1.84                     | 0.42              |
| 1:XA:690:G:H22    | 11:XK:55:LYS:HZ2   | 1.67                     | 0.42              |
| 1:XA:598:U:H4'    | 8:XH:94:TYR:CD2    | 2.55                     | 0.42              |
| 1:XA:1255:G:OP1   | 10:XJ:45:ARG:NH2   | 2.52                     | 0.42              |
| 49:Y3:8:LEU:HB3   | 49:Y3:31:LEU:HA    | 2.01                     | 0.42              |
| 19:XS:64:GLU:HG3  | 50:Y4:55:ARG:NH1   | 2.34                     | 0.42              |
| 54:Y8:52:LYS:N    | 54:Y8:53:PRO:HD2   | 2.33                     | 0.42              |
| 25:YA:1926:U:O2'  | 25:YA:1928:A:N7    | 2.46                     | 0.42              |
| 25:YA:2563:U:H1'  | 25:YA:2566:A:N6    | 2.34                     | 0.42              |
| 25:YA:2655:G:O2'  | 25:YA:2656:U:P     | 2.77                     | 0.42              |
| 25:YA:2712:U:O2'  | 25:YA:2712(A):A:C8 | 2.73                     | 0.42              |
| 25:YA:434:U:H1'   | 25:YA:435:C:H5     | 1.84                     | 0.42              |
| 25:YA:94:G:H2'    | 25:YA:95:G:O4'     | 2.19                     | 0.42              |
| 26:YB:14:U:O3'    | 26:YB:107:U:O2'    | 2.35                     | 0.42              |
| 27:YD:36:PRO:CB   | 27:YD:61:LEU:HB3   | 2.50                     | 0.42              |
| 30:YG:16:ARG:N    | 30:YG:17:PRO:HD2   | 2.34                     | 0.42              |
| 31:YH:15:VAL:HG11 | 31:YH:79:VAL:CG2   | 2.45                     | 0.42              |
| 31:YH:159:GLU:O   | 31:YH:160:LYS:HG2  | 2.19                     | 0.42              |
| 35:YP:1:MET:HB3   | 35:YP:2:LYS:H      | 1.61                     | 0.42              |
| 36:YQ:76:LYS:HG3  | 36:YQ:77:LYS:N     | 2.35                     | 0.42              |
| 36:YQ:39:PRO:HA   | 36:YQ:97:VAL:O     | 2.20                     | 0.42              |
| 38:YS:81:GLY:O    | 38:YS:83:LYS:N     | 2.53                     | 0.42              |
| 42:YW:86:LEU:HD22 | 42:YW:96:ILE:HD12  | 2.01                     | 0.42              |
| 1:QA:1162:C:H42   | 1:QA:1174:G:H1     | 1.68                     | 0.42              |
| 1:QA:1170:A:H8    | 1:QA:1170:A:O5'    | 2.02                     | 0.42              |
| 1:QA:1292:U:H2'   | 1:QA:1293:G:C8     | 2.54                     | 0.42              |
| 1:QA:464:G:C6     | 1:QA:466:C:H5'     | 2.54                     | 0.42              |
| 1:QA:514:C:H2'    | 1:QA:515:G:C8      | 2.54                     | 0.42              |
| 1:QA:707:C:H2'    | 1:QA:708:C:C6      | 2.55                     | 0.42              |
| 2:QB:92:TYR:CD1   | 2:QB:151:GLY:HA3   | 2.55                     | 0.42              |
| 6:QF:22:GLU:O     | 6:QF:26:ILE:HG13   | 2.19                     | 0.42              |
| 11:QK:41:THR:HG22 | 11:QK:42:TRP:N     | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:QO:48:LYS:HA    | 15:QO:48:LYS:HD3   | 1.76                     | 0.42              |
| 25:RA:139:G:N2     | 25:RA:141:A:N1     | 2.64                     | 0.42              |
| 25:RA:1470:G:N2    | 25:RA:1522:G:OP2   | 2.52                     | 0.42              |
| 25:RA:1641:A:H2'   | 25:RA:1642:G:O4'   | 2.20                     | 0.42              |
| 25:RA:1860:G:H2'   | 25:RA:1861:G:H8    | 1.84                     | 0.42              |
| 25:RA:2282:G:H4'   | 25:RA:2389:G:O2'   | 2.20                     | 0.42              |
| 25:RA:323:G:C2     | 25:RA:333:G:H1'    | 2.54                     | 0.42              |
| 25:RA:884:C:N3     | 25:RA:892:G:C6     | 2.87                     | 0.42              |
| 25:RA:323:G:H2'    | 29:RF:169:ASN:ND2  | 2.35                     | 0.42              |
| 30:RG:159:VAL:HG21 | 30:RG:173:LEU:HD11 | 2.00                     | 0.42              |
| 30:RG:97:ASP:HA    | 30:RG:100:TRP:HD1  | 1.85                     | 0.42              |
| 31:RH:6:ARG:HG3    | 31:RH:7:LEU:HG     | 2.01                     | 0.42              |
| 39:RT:26:ASP:HB3   | 39:RT:92:GLY:N     | 2.18                     | 0.42              |
| 40:RU:75:ASN:HB2   | 40:RU:78:THR:H     | 1.85                     | 0.42              |
| 44:RY:50:ARG:HG2   | 44:RY:50:ARG:H     | 1.67                     | 0.42              |
| 45:RZ:169:GLU:O    | 45:RZ:171:ILE:HG23 | 2.19                     | 0.42              |
| 1:XA:272:C:H2'     | 1:XA:273:A:C8      | 2.55                     | 0.42              |
| 1:XA:58:C:O2'      | 1:XA:388:G:N7      | 2.42                     | 0.42              |
| 1:XA:514:C:H2'     | 1:XA:515:G:C8      | 2.54                     | 0.42              |
| 1:XA:626:U:H2'     | 1:XA:627:G:C8      | 2.55                     | 0.42              |
| 2:XB:7:VAL:HG11    | 2:XB:217:ARG:CZ    | 2.49                     | 0.42              |
| 5:XE:131:ILE:HD13  | 5:XE:131:ILE:HA    | 1.85                     | 0.42              |
| 9:XI:32:ASP:OD1    | 9:XI:33:PHE:N      | 2.53                     | 0.42              |
| 18:XR:43:PHE:CE1   | 18:XR:58:LEU:HD11  | 2.54                     | 0.42              |
| 20:XT:50:GLU:HG3   | 20:XT:51:GLU:N     | 2.33                     | 0.42              |
| 52:Y6:15:GLU:HG2   | 52:Y6:49:HIS:NE2   | 2.34                     | 0.42              |
| 25:YA:1179:C:H2'   | 25:YA:1180:C:O4'   | 2.20                     | 0.42              |
| 25:YA:1497:U:H5''  | 25:YA:1498:C:H5    | 1.83                     | 0.42              |
| 25:YA:1803:A:O2'   | 27:YD:259:THR:HG21 | 2.18                     | 0.42              |
| 25:YA:2052:G:C4    | 25:YA:2053:G:C8    | 3.07                     | 0.42              |
| 25:YA:2647:U:H2'   | 25:YA:2648:C:C6    | 2.55                     | 0.42              |
| 27:YD:25:THR:HG22  | 27:YD:82:ILE:H     | 1.84                     | 0.42              |
| 27:YD:35:LYS:HE3   | 27:YD:64:ILE:N     | 2.35                     | 0.42              |
| 28:YE:57:LYS:HD2   | 28:YE:57:LYS:HA    | 1.87                     | 0.42              |
| 29:YF:45:ARG:HH11  | 29:YF:45:ARG:CG    | 2.33                     | 0.42              |
| 25:YA:911:A:H2'    | 36:YQ:9:TYR:OH     | 2.20                     | 0.42              |
| 1:QA:1386:G:H2'    | 1:QA:1387:G:H8     | 1.83                     | 0.42              |
| 1:QA:836:G:C6      | 1:QA:851:G:C6      | 3.08                     | 0.42              |
| 3:QC:112:SER:O     | 3:QC:116:VAL:HG23  | 2.20                     | 0.42              |
| 5:QE:47:LYS:HB2    | 5:QE:47:LYS:HE2    | 1.82                     | 0.42              |
| 12:QL:38:THR:HG21  | 12:QL:65:GLU:OE2   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:R8:4:MET:SD    | 54:R8:61:LEU:HD12 | 2.59                     | 0.42              |
| 54:R8:59:LYS:NZ   | 54:R8:59:LYS:HB2  | 2.35                     | 0.42              |
| 25:RA:1016:G:H2'  | 25:RA:1017:G:O4'  | 2.19                     | 0.42              |
| 25:RA:1794:U:H2'  | 25:RA:1795:C:H6   | 1.83                     | 0.42              |
| 25:RA:579:G:O2'   | 25:RA:2019:A:OP1  | 2.29                     | 0.42              |
| 25:RA:2422:A:H2'  | 25:RA:2424:C:C6   | 2.55                     | 0.42              |
| 25:RA:247:G:H4'   | 25:RA:386:G:C4    | 2.54                     | 0.42              |
| 25:RA:2517:C:O3'  | 25:RA:2518:A:H3'  | 2.19                     | 0.42              |
| 25:RA:456:C:O2'   | 25:RA:457:A:H5'   | 2.19                     | 0.42              |
| 25:RA:918:A:N3    | 26:RB:80:U:O2'    | 2.41                     | 0.42              |
| 30:RG:173:LEU:O   | 30:RG:178:PHE:HB2 | 2.20                     | 0.42              |
| 37:RR:63:ARG:HA   | 37:RR:80:PHE:CZ   | 2.54                     | 0.42              |
| 43:RX:44:GLU:O    | 43:RX:48:LYS:N    | 2.52                     | 0.42              |
| 43:RX:60:ARG:HH12 | 53:R7:47:ARG:NH2  | 2.12                     | 0.42              |
| 45:RZ:103:ARG:HD3 | 45:RZ:136:PHE:CG  | 2.54                     | 0.42              |
| 1:XA:1225:A:N3    | 1:XA:1225:A:H2'   | 2.35                     | 0.42              |
| 1:XA:1446:A:O2'   | 1:XA:1447:G:P     | 2.78                     | 0.42              |
| 1:XA:718:G:N2     | 18:XR:82:THR:HG23 | 2.34                     | 0.42              |
| 1:XA:792:A:O2'    | 1:XA:794:A:N7     | 2.41                     | 0.42              |
| 3:XC:32:LEU:HD22  | 3:XC:59:ARG:NH1   | 2.34                     | 0.42              |
| 3:XC:91:LEU:O     | 3:XC:95:THR:OG1   | 2.19                     | 0.42              |
| 46:Y0:53:MET:CB   | 46:Y0:59:LEU:HD23 | 2.50                     | 0.42              |
| 52:Y6:14:THR:HG21 | 52:Y6:19:ARG:HH21 | 1.85                     | 0.42              |
| 25:YA:127:A:H5''  | 25:YA:128:C:C6    | 2.54                     | 0.42              |
| 25:YA:1747:G:H2'  | 25:YA:1748:G:H8   | 1.84                     | 0.42              |
| 25:YA:1838:C:H4'  | 25:YA:1839:G:H8   | 1.84                     | 0.42              |
| 25:YA:2667:C:H1'  | 31:YH:109:PHE:CD1 | 2.55                     | 0.42              |
| 25:YA:2816:C:O2   | 25:YA:2883:A:O2'  | 2.36                     | 0.42              |
| 25:YA:71:A:N6     | 25:YA:114:U:H1'   | 2.34                     | 0.42              |
| 25:YA:787:U:H5''  | 25:YA:788:A:H5'   | 2.02                     | 0.42              |
| 38:YS:106:ARG:HA  | 38:YS:110:LEU:CD2 | 2.47                     | 0.42              |
| 38:YS:83:LYS:NZ   | 38:YS:109:GLY:HA2 | 2.33                     | 0.42              |
| 41:YV:65:GLY:O    | 41:YV:90:PRO:HA   | 2.20                     | 0.42              |
| 1:QA:1036:G:H5'   | 1:QA:1037:C:OP2   | 2.18                     | 0.42              |
| 1:QA:1264:C:H2'   | 1:QA:1265:G:C8    | 2.54                     | 0.42              |
| 1:QA:630:G:O3'    | 1:QA:631:G:H4'    | 2.19                     | 0.42              |
| 1:QA:648:A:H2'    | 1:QA:649:G:C8     | 2.55                     | 0.42              |
| 1:QA:662:G:H2'    | 1:QA:663:A:H8     | 1.84                     | 0.42              |
| 1:QA:728:A:H2'    | 1:QA:729:A:C8     | 2.55                     | 0.42              |
| 1:QA:828:A:H2'    | 1:QA:829:G:O4'    | 2.20                     | 0.42              |
| 2:QB:27:LYS:HD2   | 2:QB:193:ASP:CB   | 2.46                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:QE:79:GLU:HB3   | 5:QE:92:LYS:HA     | 2.02                     | 0.42              |
| 10:QJ:22:LYS:HB3  | 10:QJ:22:LYS:HE3   | 1.68                     | 0.42              |
| 10:QJ:76:ASN:HA   | 10:QJ:77:PRO:HD2   | 1.85                     | 0.42              |
| 15:QO:43:LEU:HA   | 15:QO:43:LEU:HD23  | 1.74                     | 0.42              |
| 17:QQ:10:VAL:HG13 | 17:QQ:19:VAL:HB    | 2.01                     | 0.42              |
| 48:R2:70:GLN:O    | 48:R2:71:ASN:HB2   | 2.19                     | 0.42              |
| 50:R4:14:ILE:HG22 | 50:R4:24:THR:HG22  | 2.01                     | 0.42              |
| 52:R6:28:ARG:HB3  | 52:R6:30:THR:H     | 1.84                     | 0.42              |
| 53:R7:47:ARG:HB2  | 53:R7:48:LYS:H     | 1.68                     | 0.42              |
| 25:RA:184:C:H2'   | 25:RA:185:U:C6     | 2.55                     | 0.42              |
| 25:RA:2021:C:OP1  | 51:R5:12:SER:OG    | 2.37                     | 0.42              |
| 25:RA:2437:U:H2'  | 25:RA:2438:U:C6    | 2.55                     | 0.42              |
| 25:RA:2729:G:H1'  | 28:RE:187:ALA:HB2  | 2.01                     | 0.42              |
| 26:RB:52:A:O2'    | 26:RB:53:A:N7      | 2.51                     | 0.42              |
| 26:RB:5:C:OP1     | 26:RB:61:G:O2'     | 2.33                     | 0.42              |
| 27:RD:96:HIS:NE2  | 27:RD:102:LYS:HE2  | 2.34                     | 0.42              |
| 25:RA:1803:A:H4'  | 27:RD:259:THR:HG23 | 2.01                     | 0.42              |
| 28:RE:78:LEU:HG   | 28:RE:79:ARG:NE    | 2.35                     | 0.42              |
| 29:RF:182:ASN:O   | 29:RF:186:ILE:HG12 | 2.20                     | 0.42              |
| 30:RG:151:ALA:HB3 | 30:RG:153:ARG:NH1  | 2.35                     | 0.42              |
| 33:RN:35:ARG:HB2  | 33:RN:42:TRP:CZ3   | 2.55                     | 0.42              |
| 1:XA:1286:A:H2'   | 1:XA:1287:A:H4'    | 2.01                     | 0.42              |
| 1:XA:1399:C:C2    | 1:XA:1502:A:N6     | 2.88                     | 0.42              |
| 1:XA:426:G:OP1    | 4:XD:36:ARG:NH1    | 2.45                     | 0.42              |
| 1:XA:89:U:HO2'    | 1:XA:90:C:P        | 2.40                     | 0.42              |
| 2:XB:223:ILE:HA   | 2:XB:226:ARG:HB3   | 2.02                     | 0.42              |
| 7:XG:15:ASP:O     | 7:XG:19:GLY:HA2    | 2.20                     | 0.42              |
| 8:XH:121:ASP:N    | 8:XH:121:ASP:OD1   | 2.47                     | 0.42              |
| 13:XM:80:ARG:HE   | 50:Y4:71:ARG:NH2   | 2.10                     | 0.42              |
| 46:Y0:27:GLU:HB2  | 46:Y0:69:PHE:CD1   | 2.53                     | 0.42              |
| 25:YA:1265:A:H8   | 25:YA:1265:A:OP1   | 2.01                     | 0.42              |
| 25:YA:2124:G:H2'  | 25:YA:2125:G:O4'   | 2.19                     | 0.42              |
| 25:YA:2378:A:H8   | 25:YA:2378:A:O5'   | 2.01                     | 0.42              |
| 25:YA:2821:A:OP1  | 28:YE:110:GLY:N    | 2.40                     | 0.42              |
| 25:YA:704:G:H2'   | 25:YA:726:G:H22    | 1.85                     | 0.42              |
| 25:YA:994:C:OP1   | 40:YU:53:ARG:NH2   | 2.52                     | 0.42              |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HA    | 2.02                     | 0.42              |
| 33:YN:46:VAL:HG13 | 33:YN:48:MET:HG3   | 2.02                     | 0.42              |
| 34:YO:21:CYS:O    | 34:YO:22:ILE:HD13  | 2.20                     | 0.42              |
| 35:YP:36:LYS:HB3  | 35:YP:40:SER:CB    | 2.49                     | 0.42              |
| 38:YS:60:GLY:O    | 38:YS:61:ASN:HB3   | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:26:ASP:HB2   | 39:YT:91:ARG:HA    | 2.00                     | 0.42              |
| 44:YY:51:VAL:HG23  | 44:YY:57:GLN:N     | 2.35                     | 0.42              |
| 25:YA:328:U:H4'    | 44:YY:68:HIS:CD2   | 2.55                     | 0.42              |
| 1:QA:389:A:H2'     | 1:QA:390:C:O4'     | 2.20                     | 0.42              |
| 1:QA:518:C:H5'     | 1:QA:530:G:O4'     | 2.20                     | 0.42              |
| 1:QA:939:G:H2'     | 1:QA:940:C:C6      | 2.55                     | 0.42              |
| 2:QB:219:VAL:O     | 2:QB:223:ILE:HG13  | 2.19                     | 0.42              |
| 2:QB:60:ASP:O      | 2:QB:64:ARG:HG2    | 2.19                     | 0.42              |
| 3:QC:134:ILE:HD11  | 3:QC:153:VAL:HG21  | 2.02                     | 0.42              |
| 3:QC:56:ASP:O      | 3:QC:66:VAL:HA     | 2.20                     | 0.42              |
| 10:QJ:81:THR:C     | 10:QJ:83:GLU:H     | 2.23                     | 0.42              |
| 13:QM:80:ARG:HB2   | 50:R4:71:ARG:NH2   | 2.35                     | 0.42              |
| 1:QA:1216:G:H5''   | 14:QN:5:ALA:HB2    | 2.02                     | 0.42              |
| 15:QO:87:ILE:HG22  | 15:QO:88:ARG:N     | 2.35                     | 0.42              |
| 1:QA:1320:C:N4     | 19:QS:36:ARG:HG3   | 2.35                     | 0.42              |
| 22:QV:28:C:H2'     | 22:QV:29:G:C8      | 2.54                     | 0.42              |
| 23:QW:57:G:H2'     | 23:QW:58:A:H5'     | 2.01                     | 0.42              |
| 47:R1:90:ILE:O     | 47:R1:94:LEU:HB2   | 2.20                     | 0.42              |
| 42:RW:34:ASN:ND2   | 51:R5:39:MET:HG3   | 2.35                     | 0.42              |
| 52:R6:45:LYS:HD3   | 52:R6:45:LYS:HA    | 1.75                     | 0.42              |
| 25:RA:1051:G:H2'   | 25:RA:1052:C:O4'   | 2.19                     | 0.42              |
| 25:RA:1479:G:H2'   | 25:RA:1480:G:O4'   | 2.20                     | 0.42              |
| 25:RA:1991:U:H2'   | 25:RA:1992:G:H5''  | 2.01                     | 0.42              |
| 25:RA:2392:A:H2    | 25:RA:2424:C:H42   | 1.65                     | 0.42              |
| 25:RA:2391:G:C6    | 25:RA:2427:C:H1'   | 2.55                     | 0.42              |
| 25:RA:467:G:OP1    | 53:R7:33:ARG:NH1   | 2.51                     | 0.42              |
| 25:RA:590:A:H2'    | 25:RA:591:C:C6     | 2.55                     | 0.42              |
| 26:RB:17:C:H2'     | 26:RB:18:G:O4'     | 2.19                     | 0.42              |
| 27:RD:245:PRO:HA   | 27:RD:246:PRO:HD3  | 1.95                     | 0.42              |
| 28:RE:21:VAL:HG23  | 28:RE:22:PRO:CG    | 2.41                     | 0.42              |
| 29:RF:28:ILE:HG13  | 29:RF:28:ILE:H     | 1.68                     | 0.42              |
| 31:RH:105:LEU:HD22 | 31:RH:113:VAL:HB   | 2.01                     | 0.42              |
| 31:RH:164:TYR:O    | 31:RH:166:GLY:N    | 2.52                     | 0.42              |
| 38:RS:14:VAL:HG11  | 38:RS:90:GLY:O     | 2.19                     | 0.42              |
| 42:RW:75:TYR:CZ    | 42:RW:104:THR:HG21 | 2.55                     | 0.42              |
| 1:XA:1189:C:OP1    | 10:XJ:51:ARG:NH2   | 2.47                     | 0.42              |
| 1:XA:1429:C:H2'    | 1:XA:1430:C:C6     | 2.55                     | 0.42              |
| 1:XA:1465:C:H2'    | 1:XA:1466:C:O4'    | 2.20                     | 0.42              |
| 1:XA:163:C:H2'     | 1:XA:164:U:C6      | 2.55                     | 0.42              |
| 1:XA:836:G:C6      | 1:XA:851:G:C6      | 3.08                     | 0.42              |
| 2:XB:113:HIS:O     | 2:XB:116:GLU:HB2   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:XI:4:TYR:CE1    | 9:XI:88:TYR:HB2   | 2.55                     | 0.42              |
| 13:XM:40:ASN:ND2  | 13:XM:43:THR:HG23 | 2.34                     | 0.42              |
| 1:XA:530:G:O6     | 24:XX:21:C:H1'    | 2.20                     | 0.42              |
| 51:Y5:31:VAL:HG13 | 51:Y5:42:PRO:HG3  | 2.01                     | 0.42              |
| 54:Y8:60:LEU:C    | 54:Y8:63:PRO:HD2  | 2.40                     | 0.42              |
| 25:YA:2168:G:H2'  | 25:YA:2168:G:N3   | 2.34                     | 0.42              |
| 25:YA:2378:A:C5   | 25:YA:2379:G:H1'  | 2.55                     | 0.42              |
| 25:YA:2698:U:H2'  | 25:YA:2699:C:C6   | 2.55                     | 0.42              |
| 25:YA:247:G:H4'   | 25:YA:386:G:C4    | 2.55                     | 0.42              |
| 25:YA:671:C:H2'   | 25:YA:672:C:C6    | 2.53                     | 0.42              |
| 35:YP:29:LYS:HD2  | 35:YP:30:THR:CG2  | 2.50                     | 0.42              |
| 25:YA:2467:C:H4'  | 36:YQ:123:HIS:CD2 | 2.54                     | 0.42              |
| 45:YZ:182:LYS:HE3 | 45:YZ:182:LYS:HB2 | 1.69                     | 0.42              |
| 45:YZ:54:HIS:ND1  | 45:YZ:99:TYR:O    | 2.47                     | 0.42              |
| 1:QA:1285:A:H1'   | 1:QA:1286:A:OP2   | 2.20                     | 0.42              |
| 1:QA:1314:C:H2'   | 1:QA:1315:U:C6    | 2.55                     | 0.42              |
| 1:QA:328:C:H4'    | 1:QA:329:A:O5'    | 2.20                     | 0.42              |
| 1:QA:596:C:H2'    | 1:QA:597:G:H8     | 1.84                     | 0.42              |
| 2:QB:88:ALA:HB2   | 2:QB:219:VAL:HG13 | 2.02                     | 0.42              |
| 4:QD:122:ARG:HD3  | 4:QD:122:ARG:O    | 2.20                     | 0.42              |
| 6:QF:15:ASP:O     | 6:QF:17:SER:N     | 2.53                     | 0.42              |
| 7:QG:13:GLN:O     | 7:QG:24:THR:HG21  | 2.20                     | 0.42              |
| 8:QH:54:ASP:O     | 8:QH:56:LYS:HG3   | 2.20                     | 0.42              |
| 11:QK:48:ILE:HG23 | 11:QK:63:LEU:HD22 | 2.01                     | 0.42              |
| 12:QL:11:VAL:HG11 | 17:QQ:36:ILE:HG21 | 2.00                     | 0.42              |
| 18:QR:53:ARG:HE   | 18:QR:59:SER:C    | 2.22                     | 0.42              |
| 49:R3:35:ARG:HB3  | 49:R3:37:LEU:HD21 | 2.01                     | 0.42              |
| 25:RA:1268:A:OP1  | 25:RA:2006:C:OP1  | 2.37                     | 0.42              |
| 25:RA:1321:A:H2'  | 25:RA:1322:A:O4'  | 2.19                     | 0.42              |
| 25:RA:2215:G:H2'  | 25:RA:2216:G:H8   | 1.85                     | 0.42              |
| 25:RA:2415:G:H5'  | 35:RP:67:MET:H    | 1.85                     | 0.42              |
| 25:RA:921:G:H4'   | 25:RA:2269:A:C5   | 2.55                     | 0.42              |
| 27:RD:35:LYS:HB3  | 27:RD:36:PRO:HA   | 2.01                     | 0.42              |
| 29:RF:184:TYR:O   | 29:RF:188:ARG:HG3 | 2.19                     | 0.42              |
| 30:RG:116:ASP:OD1 | 30:RG:116:ASP:N   | 2.53                     | 0.42              |
| 30:RG:47:LYS:HD3  | 30:RG:81:LYS:CB   | 2.49                     | 0.42              |
| 31:RH:4:ILE:HB    | 31:RH:6:ARG:HG2   | 2.01                     | 0.42              |
| 36:RQ:18:LYS:HB3  | 36:RQ:19:GLY:H    | 1.50                     | 0.42              |
| 38:RS:78:LEU:HD23 | 38:RS:78:LEU:HA   | 1.86                     | 0.42              |
| 45:RZ:94:GLU:HB2  | 45:RZ:130:PRO:HD2 | 2.02                     | 0.42              |
| 1:XA:1319:A:H5'   | 1:XA:1320:C:OP1   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1412:C:H2'   | 1:XA:1413:A:C8    | 2.55                     | 0.42              |
| 1:XA:201:C:H42    | 1:XA:216:G:H1     | 1.66                     | 0.42              |
| 1:XA:784:C:H4'    | 25:YA:1837:C:OP1  | 2.20                     | 0.42              |
| 1:XA:880:C:H5''   | 12:XL:12:ARG:HH12 | 1.85                     | 0.42              |
| 1:XA:921:U:H2'    | 1:XA:922:G:O4'    | 2.20                     | 0.42              |
| 2:XB:19:HIS:CE1   | 2:XB:206:ASP:HB2  | 2.54                     | 0.42              |
| 3:XC:85:ARG:HD2   | 3:XC:85:ARG:HA    | 1.83                     | 0.42              |
| 9:XI:125:TYR:HD1  | 9:XI:126:SER:H    | 1.68                     | 0.42              |
| 12:XL:46:LYS:HG2  | 12:XL:47:LYS:N    | 2.35                     | 0.42              |
| 13:XM:3:ARG:HG3   | 13:XM:9:ILE:HG21  | 2.01                     | 0.42              |
| 19:XS:78:ARG:HG2  | 19:XS:78:ARG:H    | 1.56                     | 0.42              |
| 51:Y5:56:LYS:CD   | 51:Y5:56:LYS:H    | 2.30                     | 0.42              |
| 35:YP:62:LEU:HD12 | 54:Y8:30:ARG:NH1  | 2.35                     | 0.42              |
| 54:Y8:44:LYS:HD2  | 54:Y8:44:LYS:N    | 2.34                     | 0.42              |
| 25:YA:1078:U:HO2' | 25:YA:1088:A:H2   | 1.63                     | 0.42              |
| 25:YA:1094:U:O2   | 25:YA:1096:A:H5'  | 2.20                     | 0.42              |
| 25:YA:814:C:O2'   | 25:YA:1225:C:N3   | 2.50                     | 0.42              |
| 25:YA:1224:G:N2   | 25:YA:1227:A:OP2  | 2.32                     | 0.42              |
| 25:YA:1794:U:H2'  | 25:YA:1795:C:H6   | 1.85                     | 0.42              |
| 25:YA:2389:G:H5'' | 25:YA:2390:U:O4'  | 2.19                     | 0.42              |
| 25:YA:2393:A:H5'  | 35:YP:62:LEU:HB3  | 2.01                     | 0.42              |
| 25:YA:2695:C:H2'  | 25:YA:2696:U:C6   | 2.55                     | 0.42              |
| 25:YA:307:G:H21   | 25:YA:330:A:N6    | 2.17                     | 0.42              |
| 25:YA:483:A:H3'   | 25:YA:484:C:C6    | 2.55                     | 0.42              |
| 25:YA:958:U:O2    | 26:YB:89(A):A:H4' | 2.20                     | 0.42              |
| 27:YD:135:PHE:CD1 | 27:YD:135:PHE:N   | 2.85                     | 0.42              |
| 27:YD:34:VAL:HG22 | 27:YD:35:LYS:HG3  | 2.00                     | 0.42              |
| 25:YA:2788:C:OP1  | 28:YE:61:ARG:NH1  | 2.53                     | 0.42              |
| 38:YS:38:GLN:HG3  | 38:YS:47:THR:HG21 | 2.02                     | 0.42              |
| 44:YY:63:LYS:HD2  | 44:YY:63:LYS:HA   | 1.86                     | 0.42              |
| 1:QA:1024:G:OP1   | 1:QA:1024:G:H4'   | 2.20                     | 0.42              |
| 1:QA:1347:G:O2'   | 1:QA:1348:U:P     | 2.78                     | 0.42              |
| 1:QA:9:G:H5''     | 5:QE:126:ARG:HE   | 1.84                     | 0.42              |
| 2:QB:184:VAL:N    | 2:QB:198:ASP:OD2  | 2.44                     | 0.42              |
| 3:QC:36:ASP:HA    | 3:QC:39:ILE:HD12  | 2.02                     | 0.42              |
| 3:QC:42:LEU:HD12  | 3:QC:42:LEU:HA    | 1.79                     | 0.42              |
| 8:QH:20:TYR:CE2   | 8:QH:75:ARG:HD2   | 2.54                     | 0.42              |
| 8:QH:12:ARG:NH1   | 8:QH:27:PRO:HD2   | 2.35                     | 0.42              |
| 9:QI:95:LYS:HZ1   | 9:QI:96:LEU:HD13  | 1.85                     | 0.42              |
| 15:QO:31:LEU:O    | 15:QO:35:ARG:HG3  | 2.20                     | 0.42              |
| 18:QR:56:THR:HB   | 18:QR:58:LEU:CD1  | 2.50                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:QS:50:ALA:HB1   | 19:QS:57:HIS:HB3  | 2.02                     | 0.42              |
| 47:R1:85:LEU:HA    | 47:R1:87:PRO:HD2  | 2.01                     | 0.42              |
| 30:RG:6:ALA:N      | 50:R4:23:GLU:HG2  | 2.31                     | 0.42              |
| 51:R5:55:ARG:CG    | 51:R5:55:ARG:NH1  | 2.79                     | 0.42              |
| 25:RA:2477:C:H2'   | 55:R9:1:MET:HG3   | 2.02                     | 0.42              |
| 25:RA:2143:C:H2'   | 25:RA:2144:U:O4'  | 2.20                     | 0.42              |
| 25:RA:2246:G:H2'   | 25:RA:2247:A:C8   | 2.55                     | 0.42              |
| 25:RA:242:G:H1'    | 25:RA:243:U:OP2   | 2.20                     | 0.42              |
| 25:RA:2469:A:OP1   | 25:RA:2469:A:H4'  | 2.20                     | 0.42              |
| 25:RA:2704:C:H2'   | 25:RA:2705:A:O4'  | 2.19                     | 0.42              |
| 25:RA:675:A:N3     | 25:RA:2443:C:O2'  | 2.45                     | 0.42              |
| 25:RA:833:U:H2'    | 25:RA:834:C:C6    | 2.55                     | 0.42              |
| 26:RB:14:U:H4'     | 26:RB:70:C:O2     | 2.20                     | 0.42              |
| 31:RH:10:PRO:HD2   | 31:RH:50:VAL:O    | 2.20                     | 0.42              |
| 35:RP:63:PRO:HA    | 54:R8:13:ARG:HB3  | 2.02                     | 0.42              |
| 39:RT:51:ARG:HG3   | 39:RT:98:LYS:HG3  | 2.02                     | 0.42              |
| 40:RU:58:ARG:NH1   | 40:RU:93:LYS:HE2  | 2.35                     | 0.42              |
| 1:XA:1179:A:H2'    | 1:XA:1180:A:O4'   | 2.19                     | 0.42              |
| 1:XA:1298:C:H4'    | 1:XA:1299:A:O4'   | 2.20                     | 0.42              |
| 1:XA:715:A:H2'     | 1:XA:716:A:C8     | 2.55                     | 0.42              |
| 11:XK:109:VAL:HG11 | 18:XR:84:LYS:HD3  | 2.02                     | 0.42              |
| 46:Y0:53:MET:HB3   | 46:Y0:59:LEU:HD23 | 2.01                     | 0.42              |
| 49:Y3:35:ARG:HB3   | 49:Y3:37:LEU:HD21 | 2.01                     | 0.42              |
| 50:Y4:16:CYS:SG    | 50:Y4:36:CYS:HB3  | 2.59                     | 0.42              |
| 50:Y4:39:CYS:O     | 50:Y4:40:HIS:HB2  | 2.20                     | 0.42              |
| 50:Y4:37:SER:HB3   | 50:Y4:42:PHE:HB3  | 2.00                     | 0.42              |
| 54:Y8:26:LYS:HB3   | 54:Y8:44:LYS:HG3  | 2.01                     | 0.42              |
| 25:YA:987:G:O2'    | 25:YA:1000:A:N3   | 2.42                     | 0.42              |
| 25:YA:1239:G:H2'   | 25:YA:1240:U:O4'  | 2.20                     | 0.42              |
| 25:YA:1598:C:H5'   | 43:YX:36:LYS:CB   | 2.48                     | 0.42              |
| 25:YA:1972:A:H2'   | 25:YA:1973:G:C8   | 2.55                     | 0.42              |
| 25:YA:2655:G:O2'   | 25:YA:2656:U:OP2  | 2.38                     | 0.42              |
| 4:QD:167:GLY:O     | 27:YD:135:PHE:CE1 | 2.73                     | 0.42              |
| 27:YD:221:VAL:HG22 | 27:YD:226:MET:CE  | 2.49                     | 0.42              |
| 27:YD:245:PRO:HA   | 27:YD:246:PRO:HD3 | 1.87                     | 0.42              |
| 27:YD:89:SER:O     | 27:YD:198:ASN:ND2 | 2.52                     | 0.42              |
| 32:YI:98:ALA:HB2   | 32:YI:111:PRO:HB3 | 2.01                     | 0.42              |
| 33:YN:35:ARG:HB2   | 33:YN:42:TRP:CZ3  | 2.55                     | 0.42              |
| 33:YN:59:LYS:HE3   | 33:YN:61:ARG:HH22 | 1.84                     | 0.42              |
| 43:YX:84:ALA:HB1   | 43:YX:85:PRO:HD2  | 2.02                     | 0.42              |
| 44:YY:96:ILE:HG13  | 44:YY:98:VAL:H    | 1.85                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:YZ:1:MET:HG2    | 45:YZ:2:GLU:H     | 1.85                     | 0.42              |
| 1:QA:1240:U:OP1    | 7:QG:119:ARG:NH2  | 2.53                     | 0.41              |
| 1:QA:222:U:H2'     | 1:QA:223:U:C6     | 2.55                     | 0.41              |
| 2:QB:69:LEU:O      | 2:QB:162:ILE:HA   | 2.19                     | 0.41              |
| 14:QN:23:ARG:NH1   | 14:QN:30:ALA:HB2  | 2.35                     | 0.41              |
| 21:QU:2:GLY:O      | 21:QU:5:ASP:N     | 2.47                     | 0.41              |
| 49:R3:7:LYS:HA     | 49:R3:33:GLN:O    | 2.20                     | 0.41              |
| 50:R4:55:ARG:O     | 50:R4:59:PHE:HB3  | 2.20                     | 0.41              |
| 25:RA:1510:A:H2'   | 25:RA:1510:A:N3   | 2.35                     | 0.41              |
| 25:RA:2245:U:H5'   | 25:RA:2246:G:H5'  | 2.02                     | 0.41              |
| 25:RA:2286:A:H4'   | 25:RA:2287:A:O4'  | 2.19                     | 0.41              |
| 25:RA:2405:G:H1'   | 25:RA:2412:A:N6   | 2.35                     | 0.41              |
| 25:RA:2461:C:H2'   | 25:RA:2462:U:C6   | 2.54                     | 0.41              |
| 25:RA:2699:C:H2'   | 25:RA:2700:C:O4'  | 2.20                     | 0.41              |
| 25:RA:611:C:H2'    | 25:RA:612:G:C8    | 2.55                     | 0.41              |
| 25:RA:784:A:O4'    | 27:RD:227:ASN:ND2 | 2.53                     | 0.41              |
| 27:RD:101:GLU:OE1  | 27:RD:103:ARG:NH1 | 2.53                     | 0.41              |
| 27:RD:61:LEU:HA    | 27:RD:61:LEU:HD12 | 1.77                     | 0.41              |
| 28:RE:188:VAL:HG23 | 28:RE:189:PRO:HD2 | 2.01                     | 0.41              |
| 29:RF:129:PHE:O    | 29:RF:130:ALA:HB3 | 2.20                     | 0.41              |
| 29:RF:93:LYS:HB3   | 29:RF:94:PRO:HD2  | 2.01                     | 0.41              |
| 25:RA:2313:C:H5''  | 30:RG:91:ARG:HD3  | 2.01                     | 0.41              |
| 31:RH:125:VAL:HG13 | 31:RH:126:PRO:HG3 | 2.01                     | 0.41              |
| 34:RO:7:TYR:CE1    | 34:RO:20:MET:HB2  | 2.55                     | 0.41              |
| 4:XD:131:ARG:HG2   | 4:XD:131:ARG:H    | 1.67                     | 0.41              |
| 4:XD:127:THR:HA    | 4:XD:132:ARG:HA   | 2.02                     | 0.41              |
| 12:XL:62:SER:HB2   | 12:XL:64:TYR:CD1  | 2.55                     | 0.41              |
| 13:XM:121:LYS:HD3  | 13:XM:121:LYS:HA  | 1.91                     | 0.41              |
| 13:XM:16:ASP:HB3   | 13:XM:41:PRO:HB3  | 2.02                     | 0.41              |
| 16:XP:23:ASP:O     | 16:XP:26:ARG:HB2  | 2.20                     | 0.41              |
| 9:XI:128:ARG:NH2   | 22:XV:35:A:OP2    | 2.53                     | 0.41              |
| 23:XW:49:C:C2      | 23:XW:65:G:N2     | 2.87                     | 0.41              |
| 50:Y4:24:THR:OG1   | 50:Y4:25:TYR:N    | 2.53                     | 0.41              |
| 50:Y4:68:ARG:HB2   | 50:Y4:69:LYS:H    | 1.51                     | 0.41              |
| 25:YA:1336:A:H2'   | 25:YA:1337:G:C8   | 2.55                     | 0.41              |
| 25:YA:1499:C:H2'   | 25:YA:1500:G:H8   | 1.84                     | 0.41              |
| 25:YA:1614:A:N6    | 42:YW:88:ARG:H    | 2.18                     | 0.41              |
| 25:YA:2610:C:H4'   | 25:YA:2611:U:H5'  | 2.02                     | 0.41              |
| 25:YA:2832:U:H4'   | 25:YA:2833:G:C5'  | 2.49                     | 0.41              |
| 27:YD:232:PRO:HB3  | 27:YD:244:ARG:CZ  | 2.50                     | 0.41              |
| 28:YE:167:VAL:HG21 | 28:YE:187:ALA:HB1 | 2.01                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:YG:165:THR:OG1  | 30:YG:168:GLU:HG3 | 2.20                     | 0.41              |
| 30:YG:86:MET:HA    | 30:YG:87:PRO:HD2  | 1.95                     | 0.41              |
| 31:YH:30:LYS:HE2   | 31:YH:81:GLU:H    | 1.85                     | 0.41              |
| 32:YI:56:LYS:HZ1   | 32:YI:60:GLU:HG2  | 1.85                     | 0.41              |
| 33:YN:137:LYS:HD2  | 33:YN:137:LYS:HA  | 1.77                     | 0.41              |
| 33:YN:7:LYS:H      | 33:YN:7:LYS:HD2   | 1.84                     | 0.41              |
| 36:YQ:54:MET:HB3   | 36:YQ:64:ILE:HD13 | 2.01                     | 0.41              |
| 36:YQ:85:LYS:O     | 36:YQ:86:GLY:C    | 2.58                     | 0.41              |
| 37:YR:3:HIS:O      | 37:YR:5:LYS:N     | 2.53                     | 0.41              |
| 45:YZ:157:LEU:HD22 | 45:YZ:161:VAL:HB  | 2.02                     | 0.41              |
| 1:QA:514:C:H2'     | 1:QA:515:G:H8     | 1.85                     | 0.41              |
| 1:QA:826:C:H2'     | 1:QA:827:U:O2     | 2.20                     | 0.41              |
| 1:QA:992:U:O2      | 1:QA:993:G:N2     | 2.53                     | 0.41              |
| 2:QB:104:ASN:OD1   | 2:QB:107:THR:OG1  | 2.30                     | 0.41              |
| 8:QH:38:ILE:HD12   | 8:QH:118:VAL:HG12 | 2.02                     | 0.41              |
| 8:QH:36:LEU:HD12   | 8:QH:59:LEU:HD13  | 2.02                     | 0.41              |
| 8:QH:59:LEU:O      | 8:QH:61:VAL:HG23  | 2.21                     | 0.41              |
| 20:QT:84:LEU:HD23  | 20:QT:84:LEU:HA   | 1.86                     | 0.41              |
| 46:R0:23:VAL:HA    | 46:R0:38:VAL:HG22 | 2.00                     | 0.41              |
| 22:QV:0:C:O2'      | 46:R0:6:GLY:O     | 2.33                     | 0.41              |
| 54:R8:23:VAL:CG1   | 54:R8:46:ARG:HD3  | 2.49                     | 0.41              |
| 25:RA:1309:G:P     | 53:R7:9:ARG:HD3   | 2.60                     | 0.41              |
| 25:RA:1694:C:H4'   | 25:RA:1695:G:O5'  | 2.19                     | 0.41              |
| 27:RD:43:ARG:HB2   | 27:RD:54:ARG:HB2  | 2.02                     | 0.41              |
| 28:RE:76:ARG:HD2   | 28:RE:76:ARG:N    | 2.35                     | 0.41              |
| 29:RF:46:ARG:HH11  | 29:RF:46:ARG:HG2  | 1.84                     | 0.41              |
| 25:RA:2305:A:O5'   | 30:RG:134:GLY:HA3 | 2.19                     | 0.41              |
| 32:RI:135:GLU:HB2  | 32:RI:136:VAL:H   | 1.77                     | 0.41              |
| 33:RN:10:GLU:HA    | 33:RN:11:PRO:HD3  | 1.65                     | 0.41              |
| 36:RQ:17:LEU:HD21  | 36:RQ:41:TRP:HD1  | 1.84                     | 0.41              |
| 36:RQ:68:ILE:HD13  | 36:RQ:103:MET:HG2 | 2.02                     | 0.41              |
| 26:RB:7:G:H5'      | 38:RS:29:PHE:CE2  | 2.55                     | 0.41              |
| 1:XA:1327:C:H2'    | 1:XA:1328:C:C6    | 2.55                     | 0.41              |
| 1:XA:41:G:H2'      | 1:XA:42:G:C8      | 2.55                     | 0.41              |
| 1:XA:608:A:H2'     | 1:XA:609:A:O4'    | 2.20                     | 0.41              |
| 1:XA:966:G:O2'     | 9:XI:127:LYS:O    | 2.38                     | 0.41              |
| 4:XD:120:LEU:HD23  | 4:XD:120:LEU:HA   | 1.88                     | 0.41              |
| 10:XJ:3:LYS:HB2    | 10:XJ:75:ILE:O    | 2.19                     | 0.41              |
| 13:XM:12:ASN:N     | 13:XM:45:VAL:HG13 | 2.35                     | 0.41              |
| 13:XM:20:THR:O     | 13:XM:22:ILE:N    | 2.52                     | 0.41              |
| 16:XP:17:TYR:HE2   | 16:XP:41:PRO:HG3  | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:XP:56:ALA:HB1   | 16:XP:74:LEU:HD13  | 2.02                     | 0.41              |
| 18:XR:38:GLU:O     | 18:XR:42:ARG:NH1   | 2.53                     | 0.41              |
| 46:Y0:36:ILE:HD11  | 46:Y0:39:ARG:HG2   | 2.02                     | 0.41              |
| 46:Y0:41:ARG:HA    | 46:Y0:41:ARG:NE    | 2.34                     | 0.41              |
| 47:Y1:76:ARG:H     | 47:Y1:76:ARG:HD2   | 1.84                     | 0.41              |
| 25:YA:2059:A:H5'   | 25:YA:2060:A:OP2   | 2.20                     | 0.41              |
| 25:YA:2745:C:C4    | 25:YA:2746:U:C4    | 3.08                     | 0.41              |
| 26:YB:95:U:H2'     | 26:YB:96:G:C8      | 2.54                     | 0.41              |
| 25:YA:2619:C:H4'   | 28:YE:151:TYR:O    | 2.20                     | 0.41              |
| 29:YF:107:LYS:CD   | 29:YF:207:GLY:H    | 2.30                     | 0.41              |
| 33:YN:29:LYS:H     | 33:YN:29:LYS:HG2   | 1.53                     | 0.41              |
| 33:YN:65:LYS:O     | 33:YN:69:GLN:HG2   | 2.20                     | 0.41              |
| 35:YP:82:GLY:HA3   | 35:YP:115:LEU:HD21 | 2.01                     | 0.41              |
| 37:YR:2:ARG:HG2    | 37:YR:5:LYS:NZ     | 2.35                     | 0.41              |
| 38:YS:51:ALA:HB1   | 38:YS:69:VAL:HG23  | 2.02                     | 0.41              |
| 40:YU:109:LEU:HD23 | 40:YU:109:LEU:HA   | 1.89                     | 0.41              |
| 40:YU:30:LYS:HA    | 40:YU:30:LYS:HD3   | 1.90                     | 0.41              |
| 25:YA:1188:U:H4'   | 41:YV:79:VAL:HG22  | 2.01                     | 0.41              |
| 43:YX:26:TYR:HB3   | 43:YX:92:LEU:HD12  | 2.02                     | 0.41              |
| 1:QA:1241:G:H2'    | 1:QA:1242:C:C6     | 2.55                     | 0.41              |
| 1:QA:414:A:OP2     | 1:QA:428:G:N2      | 2.33                     | 0.41              |
| 2:QB:120:ALA:C     | 2:QB:122:PHE:H     | 2.23                     | 0.41              |
| 2:QB:208:ILE:HA    | 2:QB:211:ILE:HD12  | 2.02                     | 0.41              |
| 2:QB:210:SER:O     | 2:QB:214:ILE:HG12  | 2.21                     | 0.41              |
| 4:QD:173:TRP:CD1   | 4:QD:174:LEU:HG    | 2.55                     | 0.41              |
| 8:QH:51:VAL:HG21   | 8:QH:60:ARG:HG2    | 2.02                     | 0.41              |
| 12:QL:103:GLY:N    | 12:QL:107:ALA:O    | 2.49                     | 0.41              |
| 17:QQ:83:ASP:O     | 17:QQ:87:LYS:HG2   | 2.20                     | 0.41              |
| 53:R7:1:MET:SD     | 53:R7:3:ARG:NH2    | 2.93                     | 0.41              |
| 25:RA:1366:A:H2'   | 25:RA:1367:A:O4'   | 2.19                     | 0.41              |
| 25:RA:1506:C:H3'   | 25:RA:1507:A:H5''  | 2.02                     | 0.41              |
| 25:RA:1543:A:N3    | 25:RA:1545:A:N9    | 2.68                     | 0.41              |
| 22:QV:75:C:OP1     | 25:RA:2602:A:OP1   | 2.38                     | 0.41              |
| 29:RF:177:ALA:HB1  | 29:RF:178:PRO:HD2  | 2.03                     | 0.41              |
| 35:RP:20:GLY:HA2   | 35:RP:27:HIS:O     | 2.19                     | 0.41              |
| 35:RP:81:GLN:HG2   | 35:RP:106:LEU:HD23 | 2.02                     | 0.41              |
| 37:RR:109:ALA:HA   | 37:RR:110:PRO:HD2  | 1.95                     | 0.41              |
| 37:RR:22:ARG:HA    | 37:RR:47:PHE:HE2   | 1.86                     | 0.41              |
| 38:RS:108:GLY:O    | 38:RS:110:LEU:HG   | 2.20                     | 0.41              |
| 41:RV:76:LYS:HB2   | 41:RV:81:TYR:HB3   | 2.01                     | 0.41              |
| 45:RZ:110:GLY:HA2  | 45:RZ:111:VAL:O    | 2.19                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1391:U:H2'    | 1:XA:1392:G:C8     | 2.55                     | 0.41              |
| 1:XA:381:C:H2'     | 1:XA:382:A:O4'     | 2.20                     | 0.41              |
| 1:XA:485:G:O2'     | 1:XA:486:U:P       | 2.79                     | 0.41              |
| 1:XA:883:C:N4      | 1:XA:884:U:O4      | 2.54                     | 0.41              |
| 1:XA:925:G:H1'     | 1:XA:1502:A:C4     | 2.55                     | 0.41              |
| 1:XA:980:C:H3'     | 1:XA:981:U:H6      | 1.85                     | 0.41              |
| 1:XA:878:G:P       | 8:XH:88:LYS:HD2    | 2.59                     | 0.41              |
| 6:XF:97:PHE:N      | 18:XR:30:ASP:OD1   | 2.54                     | 0.41              |
| 1:XA:191:G:C4      | 20:XT:105:SER:HB3  | 2.55                     | 0.41              |
| 47:Y1:89:GLU:HA    | 47:Y1:93:GLU:HB2   | 2.02                     | 0.41              |
| 25:YA:1825:A:OP1   | 27:YD:231:HIS:NE2  | 2.53                     | 0.41              |
| 25:YA:2081:C:H2'   | 25:YA:2082:A:C8    | 2.55                     | 0.41              |
| 25:YA:2267:A:H5''  | 25:YA:2268:A:H5'   | 2.02                     | 0.41              |
| 25:YA:2593:U:H2'   | 25:YA:2594:C:C6    | 2.55                     | 0.41              |
| 25:YA:2857:G:N2    | 25:YA:2859:G:H3'   | 2.36                     | 0.41              |
| 27:YD:105:ILE:HD12 | 27:YD:105:ILE:HA   | 1.55                     | 0.41              |
| 29:YF:117:ARG:HD2  | 29:YF:120:GLU:OE2  | 2.20                     | 0.41              |
| 31:YH:8:PRO:HB2    | 31:YH:9:ILE:H      | 1.71                     | 0.41              |
| 32:YI:133:HIS:HB2  | 32:YI:134:PRO:CD   | 2.50                     | 0.41              |
| 32:YI:67:ARG:NH2   | 32:YI:68:LEU:HB2   | 2.33                     | 0.41              |
| 33:YN:18:ALA:HB3   | 33:YN:55:VAL:O     | 2.19                     | 0.41              |
| 41:YV:72:VAL:HG13  | 41:YV:85:LYS:HG2   | 2.01                     | 0.41              |
| 44:YY:84:ARG:O     | 44:YY:95:LYS:HD3   | 2.20                     | 0.41              |
| 45:YZ:150:LEU:HD22 | 45:YZ:171:ILE:HB   | 2.02                     | 0.41              |
| 1:QA:1367:C:OP2    | 9:QL:112:LYS:NZ    | 2.51                     | 0.41              |
| 1:QA:156:G:H2'     | 1:QA:157:G:H8      | 1.85                     | 0.41              |
| 1:QA:300:A:O5'     | 1:QA:300:A:H8      | 2.03                     | 0.41              |
| 1:QA:973:G:H3'     | 1:QA:974:A:H5''    | 2.02                     | 0.41              |
| 1:QA:1298:C:H41    | 7:QG:114:ARG:HB3   | 1.85                     | 0.41              |
| 8:QH:54:ASP:N      | 8:QH:54:ASP:OD1    | 2.53                     | 0.41              |
| 11:QK:99:GLN:HG2   | 11:QK:105:VAL:HG21 | 2.03                     | 0.41              |
| 14:QN:4:LYS:O      | 14:QN:7:ILE:HG12   | 2.20                     | 0.41              |
| 16:QP:53:VAL:O     | 16:QP:57:ARG:HG2   | 2.21                     | 0.41              |
| 25:RA:839:U:H1'    | 25:RA:1191:G:H1'   | 2.02                     | 0.41              |
| 25:RA:1259:G:H2'   | 25:RA:1260:G:C8    | 2.55                     | 0.41              |
| 25:RA:2298:A:H2'   | 25:RA:2299:G:O4'   | 2.21                     | 0.41              |
| 25:RA:2702:U:O2    | 25:RA:2702:U:H2'   | 2.20                     | 0.41              |
| 25:RA:669:G:H2'    | 25:RA:669:G:N3     | 2.36                     | 0.41              |
| 25:RA:464:U:C2     | 25:RA:788:A:C6     | 3.09                     | 0.41              |
| 25:RA:847:U:O4     | 25:RA:933:A:C6     | 2.70                     | 0.41              |
| 29:RF:113:ALA:HB1  | 29:RF:186:ILE:HG21 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:164:ARG:HG3  | 29:RF:175:THR:OG1  | 2.20                     | 0.41              |
| 30:RG:6:ALA:HB3    | 30:RG:104:GLU:OE2  | 2.20                     | 0.41              |
| 36:RQ:58:PHE:HD1   | 36:RQ:61:GLY:HA3   | 1.85                     | 0.41              |
| 38:RS:14:VAL:HG21  | 38:RS:89:ARG:HG2   | 2.02                     | 0.41              |
| 44:RY:88:LYS:HA    | 44:RY:88:LYS:NZ    | 2.35                     | 0.41              |
| 1:XA:1161:C:H2'    | 1:XA:1162:C:C6     | 2.56                     | 0.41              |
| 1:XA:149:A:H2'     | 1:XA:150:C:C6      | 2.55                     | 0.41              |
| 1:XA:303:A:H2'     | 1:XA:304:U:O4'     | 2.21                     | 0.41              |
| 1:XA:411:A:C8      | 1:XA:413:G:H1'     | 2.55                     | 0.41              |
| 3:XC:150:LYS:HE3   | 3:XC:167:TRP:HE1   | 1.84                     | 0.41              |
| 5:XE:69:VAL:HA     | 5:XE:70:PRO:HD2    | 1.76                     | 0.41              |
| 8:XH:104:ARG:HD2   | 8:XH:138:TRP:CG    | 2.56                     | 0.41              |
| 9:XI:125:TYR:HD1   | 9:XI:126:SER:N     | 2.18                     | 0.41              |
| 9:XI:40:LEU:O      | 9:XI:42:ARG:N      | 2.48                     | 0.41              |
| 11:XK:18:ARG:HA    | 11:XK:81:ASP:H     | 1.86                     | 0.41              |
| 11:XK:88:GLY:C     | 11:XK:90:GLY:H     | 2.23                     | 0.41              |
| 1:XA:1358:U:OP1    | 14:XN:35:ARG:HG3   | 2.20                     | 0.41              |
| 19:XS:40:ILE:CG1   | 19:XS:41:VAL:HG13  | 2.47                     | 0.41              |
| 20:XT:53:LEU:HD12  | 20:XT:100:ILE:HG23 | 2.02                     | 0.41              |
| 46:Y0:72:ARG:HB2   | 46:Y0:75:LEU:HB2   | 2.02                     | 0.41              |
| 25:YA:1153:C:H2'   | 25:YA:1154:G:O4'   | 2.20                     | 0.41              |
| 25:YA:270(V):G:H2' | 25:YA:270(W):G:H8  | 1.84                     | 0.41              |
| 25:YA:2849:U:H5    | 39:YT:93:ARG:NH1   | 2.14                     | 0.41              |
| 25:YA:724:U:H2'    | 25:YA:725:G:O4'    | 2.20                     | 0.41              |
| 25:YA:636:G:OP1    | 35:YP:132:LYS:HB2  | 2.20                     | 0.41              |
| 36:YQ:19:GLY:O     | 36:YQ:21:THR:OG1   | 2.23                     | 0.41              |
| 38:YS:56:LEU:HA    | 38:YS:56:LEU:HD12  | 1.76                     | 0.41              |
| 41:YV:22:VAL:HG12  | 41:YV:23:GLU:H     | 1.85                     | 0.41              |
| 41:YV:38:LEU:O     | 41:YV:51:VAL:HA    | 2.20                     | 0.41              |
| 51:R5:3:LYS:HE2    | 56:Z7:1:T17:H1     | 2.03                     | 0.41              |
| 1:QA:105:G:H2'     | 1:QA:106:C:C6      | 2.55                     | 0.41              |
| 1:QA:1119:C:H2'    | 1:QA:1120:G:C8     | 2.56                     | 0.41              |
| 1:QA:1130:A:O2'    | 9:QI:3:GLN:NE2     | 2.41                     | 0.41              |
| 1:QA:1151:A:H2'    | 1:QA:1152:A:H8     | 1.85                     | 0.41              |
| 1:QA:162:A:C5      | 1:QA:163:C:H1'     | 2.55                     | 0.41              |
| 1:QA:181:G:O2'     | 1:QA:182:U:P       | 2.79                     | 0.41              |
| 1:QA:779:C:H2'     | 1:QA:780:A:O4'     | 2.21                     | 0.41              |
| 1:QA:838:G:C5      | 1:QA:842:C:H1'     | 2.54                     | 0.41              |
| 1:QA:859:A:H2'     | 1:QA:860:A:O4'     | 2.20                     | 0.41              |
| 14:QN:29:ARG:HG2   | 14:QN:31:ARG:O     | 2.20                     | 0.41              |
| 15:QO:4:THR:HB     | 15:QO:6:GLU:CD     | 2.41                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:QS:28:LYS:HA   | 19:QS:47:HIS:HE1   | 1.86                     | 0.41              |
| 20:QT:89:ARG:HH21 | 20:QT:104:LEU:HG   | 1.85                     | 0.41              |
| 52:R6:13:CYS:O    | 52:R6:21:TYR:HA    | 2.20                     | 0.41              |
| 25:RA:1130:U:O2'  | 25:RA:1131:G:P     | 2.79                     | 0.41              |
| 25:RA:1204:A:H1'  | 25:RA:1206:G:C4    | 2.55                     | 0.41              |
| 25:RA:1297:C:H2'  | 25:RA:1298:C:H6    | 1.85                     | 0.41              |
| 25:RA:1812:A:H2'  | 25:RA:1813:G:H8    | 1.84                     | 0.41              |
| 25:RA:2150:U:H2'  | 25:RA:2151:G:H8    | 1.84                     | 0.41              |
| 25:RA:2554:U:H2'  | 25:RA:2555:U:C6    | 2.55                     | 0.41              |
| 25:RA:2665:A:H2'  | 25:RA:2666:C:O4'   | 2.21                     | 0.41              |
| 25:RA:2712:U:O2'  | 25:RA:2712(A):A:C8 | 2.72                     | 0.41              |
| 25:RA:27:G:HO2'   | 25:RA:28:A:P       | 2.42                     | 0.41              |
| 25:RA:592:G:H1    | 25:RA:665:C:H42    | 1.68                     | 0.41              |
| 27:RD:257:LEU:HA  | 27:RD:257:LEU:HD23 | 1.90                     | 0.41              |
| 27:RD:35:LYS:HE3  | 27:RD:63:ARG:C     | 2.41                     | 0.41              |
| 29:RF:178:PRO:HB2 | 29:RF:201:VAL:CG1  | 2.51                     | 0.41              |
| 30:RG:124:SER:HB2 | 30:RG:131:TYR:CE1  | 2.56                     | 0.41              |
| 30:RG:27:ASN:HB3  | 30:RG:30:GLU:HG3   | 2.01                     | 0.41              |
| 30:RG:98:ARG:HE   | 30:RG:98:ARG:HB2   | 1.38                     | 0.41              |
| 25:RA:2415:G:C5'  | 35:RP:67:MET:H     | 2.34                     | 0.41              |
| 36:RQ:40:ALA:O    | 36:RQ:42:ILE:HD12  | 2.21                     | 0.41              |
| 43:RX:40:LYS:C    | 43:RX:42:ALA:H     | 2.23                     | 0.41              |
| 44:RY:84:ARG:HD3  | 44:RY:86:ARG:NH1   | 2.35                     | 0.41              |
| 45:RZ:99:TYR:HB3  | 45:RZ:123:ASP:HB2  | 2.03                     | 0.41              |
| 1:XA:765:G:N2     | 1:XA:813:U:OP2     | 2.54                     | 0.41              |
| 2:XB:80:ILE:HD11  | 2:XB:208:ILE:HG12  | 2.02                     | 0.41              |
| 9:XI:46:ALA:HB2   | 9:XI:74:ILE:HG23   | 2.02                     | 0.41              |
| 18:XR:85:LEU:HD23 | 18:XR:88:LYS:HD2   | 2.03                     | 0.41              |
| 50:Y4:48:ARG:NH1  | 50:Y4:52:THR:H     | 2.19                     | 0.41              |
| 25:YA:1541:U:H2'  | 25:YA:1542:G:O4'   | 2.20                     | 0.41              |
| 25:YA:1588:C:H2'  | 25:YA:1589:C:H6    | 1.85                     | 0.41              |
| 25:YA:1667:G:OP2  | 25:YA:1667:G:H8    | 2.03                     | 0.41              |
| 25:YA:185:U:H4'   | 25:YA:218:A:H4'    | 2.01                     | 0.41              |
| 25:YA:752:A:H4'   | 25:YA:753:C:H5'    | 2.03                     | 0.41              |
| 28:YE:181:LEU:HA  | 28:YE:181:LEU:HD13 | 1.85                     | 0.41              |
| 30:YG:166:ASP:OD1 | 30:YG:166:ASP:N    | 2.54                     | 0.41              |
| 25:YA:1007:C:H4'  | 33:YN:108:PRO:HD3  | 2.02                     | 0.41              |
| 38:YS:88:ASP:O    | 38:YS:89:ARG:HB3   | 2.21                     | 0.41              |
| 40:YU:69:CYS:HB3  | 40:YU:106:PHE:CZ   | 2.56                     | 0.41              |
| 41:YV:72:VAL:CG1  | 41:YV:85:LYS:HG2   | 2.50                     | 0.41              |
| 1:QA:1459:C:H2'   | 1:QA:1460:A:C8     | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:74:C:H42     | 1:QA:96:G:H1       | 1.69                     | 0.41              |
| 2:QB:47:THR:HA    | 2:QB:202:PRO:HG2   | 2.00                     | 0.41              |
| 3:QC:122:GLU:HA   | 3:QC:125:GLU:OE1   | 2.21                     | 0.41              |
| 7:QG:45:ASP:O     | 7:QG:48:LYS:HB3    | 2.21                     | 0.41              |
| 12:QL:11:VAL:HG13 | 17:QQ:29:HIS:CD2   | 2.55                     | 0.41              |
| 1:QA:1227:A:O3'   | 13:QM:115:LYS:HE3  | 2.20                     | 0.41              |
| 13:QM:91:ARG:HB2  | 13:QM:98:VAL:HG13  | 2.03                     | 0.41              |
| 22:QV:76:A:O2'    | 25:RA:2451:A:O2'   | 2.21                     | 0.41              |
| 23:QW:35:A:N6     | 23:QW:36:A:N1      | 2.68                     | 0.41              |
| 25:RA:1190:G:OP1  | 35:RP:30:THR:OG1   | 2.20                     | 0.41              |
| 25:RA:1636:C:H2'  | 25:RA:1637:A:H8    | 1.82                     | 0.41              |
| 25:RA:1921:G:H2'  | 25:RA:1922:G:H8    | 1.86                     | 0.41              |
| 25:RA:512:G:H1'   | 25:RA:513:A:OP2    | 2.18                     | 0.41              |
| 25:RA:705:A:H2'   | 25:RA:706:A:O4'    | 2.20                     | 0.41              |
| 25:RA:820:A:H1'   | 25:RA:943:U:H1'    | 2.02                     | 0.41              |
| 29:RF:29:ASN:O    | 29:RF:112:MET:HE1  | 2.21                     | 0.41              |
| 33:RN:47:ALA:HB2  | 33:RN:112:LEU:HD11 | 2.02                     | 0.41              |
| 43:RX:51:VAL:HG13 | 43:RX:81:VAL:HG23  | 2.03                     | 0.41              |
| 44:RY:54:LYS:HB3  | 44:RY:55:TYR:CE1   | 2.55                     | 0.41              |
| 1:XA:564:C:H5'    | 17:XQ:32:TYR:CE1   | 2.56                     | 0.41              |
| 1:XA:748:C:H1'    | 1:XA:749:C:H5      | 1.86                     | 0.41              |
| 5:XE:79:GLU:H     | 5:XE:79:GLU:HG3    | 1.45                     | 0.41              |
| 8:XH:44:PHE:HE2   | 8:XH:109:ILE:CG2   | 2.34                     | 0.41              |
| 11:XK:48:ILE:HD13 | 11:XK:48:ILE:HA    | 1.83                     | 0.41              |
| 16:XP:8:ARG:C     | 16:XP:9:PHE:HD1    | 2.24                     | 0.41              |
| 53:Y7:47:ARG:HE   | 53:Y7:47:ARG:HB2   | 1.58                     | 0.41              |
| 55:Y9:2:LYS:HA    | 55:Y9:2:LYS:HD2    | 1.86                     | 0.41              |
| 25:YA:1103:A:H5'  | 25:YA:1104:C:C5    | 2.55                     | 0.41              |
| 25:YA:2308:G:HO2' | 25:YA:2310:A:H2    | 1.68                     | 0.41              |
| 25:YA:1759:A:H1'  | 25:YA:2711:A:C2    | 2.55                     | 0.41              |
| 28:YE:144:ARG:HB3 | 28:YE:145:LYS:H    | 1.45                     | 0.41              |
| 28:YE:25:VAL:HG11 | 39:YT:11:GLU:HG2   | 2.01                     | 0.41              |
| 29:YF:125:LEU:HA  | 29:YF:194:MET:O    | 2.20                     | 0.41              |
| 31:YH:19:VAL:HG22 | 31:YH:24:VAL:HG12  | 2.03                     | 0.41              |
| 32:YI:57:ARG:O    | 32:YI:61:ARG:HG2   | 2.20                     | 0.41              |
| 45:YZ:106:GLY:O   | 45:YZ:141:VAL:HG13 | 2.20                     | 0.41              |
| 1:QA:1043:C:H2'   | 1:QA:1044:A:C8     | 2.56                     | 0.41              |
| 1:QA:1053:G:N7    | 1:QA:1200:C:H5''   | 2.36                     | 0.41              |
| 1:QA:1327:C:H2'   | 1:QA:1328:C:C6     | 2.56                     | 0.41              |
| 1:QA:1450:U:O2'   | 1:QA:1451:A:N7     | 2.53                     | 0.41              |
| 1:QA:1522:U:H2'   | 1:QA:1523:G:H8     | 1.86                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:357:G:O3'    | 32:YI:121:LYS:NZ   | 2.53                     | 0.41              |
| 1:QA:662:G:O2'    | 1:QA:836:G:OP1     | 2.35                     | 0.41              |
| 5:QE:110:LEU:HD13 | 5:QE:118:ILE:HG12  | 2.01                     | 0.41              |
| 9:QI:40:LEU:HD11  | 9:QI:70:LYS:HG2    | 2.02                     | 0.41              |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CD2   | 2.56                     | 0.41              |
| 19:QS:67:VAL:HB   | 50:R4:59:PHE:CE1   | 2.45                     | 0.41              |
| 25:RA:1259:G:H2'  | 25:RA:1260:G:H8    | 1.86                     | 0.41              |
| 25:RA:709:U:H2'   | 25:RA:710:G:H8     | 1.86                     | 0.41              |
| 25:RA:868:U:H2'   | 25:RA:869:G:O4'    | 2.20                     | 0.41              |
| 25:RA:945:A:C4    | 25:RA:2448:A:C2    | 3.08                     | 0.41              |
| 25:RA:947:G:H2'   | 25:RA:948:G:H8     | 1.85                     | 0.41              |
| 28:RE:92:THR:HB   | 28:RE:93:VAL:H     | 1.55                     | 0.41              |
| 30:RG:47:LYS:HE3  | 30:RG:47:LYS:HB2   | 1.81                     | 0.41              |
| 37:RR:10:LEU:O    | 37:RR:12:ARG:HG3   | 2.21                     | 0.41              |
| 40:RU:61:TRP:O    | 40:RU:65:ILE:HG13  | 2.21                     | 0.41              |
| 1:XA:324:G:N1     | 1:XA:327:A:OP2     | 2.54                     | 0.41              |
| 3:XC:119:ARG:HH21 | 3:XC:140:ARG:CZ    | 2.34                     | 0.41              |
| 4:XD:52:SER:O     | 4:XD:55:ALA:HB3    | 2.21                     | 0.41              |
| 6:XF:25:ILE:HD13  | 6:XF:28:ARG:NH1    | 2.36                     | 0.41              |
| 6:XF:46:ARG:HB3   | 6:XF:60:PHE:CE1    | 2.55                     | 0.41              |
| 10:XJ:3:LYS:HD2   | 10:XJ:77:PRO:HD3   | 2.01                     | 0.41              |
| 17:XQ:59:ILE:HB   | 17:XQ:71:PHE:HB3   | 2.03                     | 0.41              |
| 17:XQ:62:SER:CB   | 17:XQ:72:ARG:HE    | 2.33                     | 0.41              |
| 20:XT:39:LYS:HG3  | 20:XT:39:LYS:H     | 1.63                     | 0.41              |
| 25:YA:1506:C:H3'  | 25:YA:1507:A:H5''  | 2.01                     | 0.41              |
| 25:YA:1773:A:H2'  | 25:YA:1774:C:O4'   | 2.19                     | 0.41              |
| 25:YA:1929:G:H4'  | 25:YA:1930:G:OP1   | 2.21                     | 0.41              |
| 25:YA:2455:G:H2'  | 25:YA:2456:C:C6    | 2.55                     | 0.41              |
| 25:YA:658:C:H2'   | 25:YA:659:C:C6     | 2.56                     | 0.41              |
| 25:YA:979:G:H2'   | 25:YA:982:C:N4     | 2.36                     | 0.41              |
| 26:YB:40:U:H3     | 26:YB:43:C:H5''    | 1.86                     | 0.41              |
| 29:YF:9:ILE:HD11  | 29:YF:125:LEU:HG   | 2.03                     | 0.41              |
| 35:YP:101:VAL:C   | 35:YP:103:ALA:H    | 2.23                     | 0.41              |
| 38:YS:107:GLU:N   | 38:YS:110:LEU:HD11 | 2.36                     | 0.41              |
| 40:YU:98:LEU:HD23 | 40:YU:99:ALA:N     | 2.36                     | 0.41              |
| 45:YZ:5:LEU:HB3   | 45:YZ:6:LYS:H      | 1.65                     | 0.41              |
| 1:QA:1120:G:H2'   | 1:QA:1121:U:C6     | 2.55                     | 0.41              |
| 1:QA:179:A:H2'    | 1:QA:180:U:C6      | 2.55                     | 0.41              |
| 1:QA:661:G:H1     | 1:QA:744:C:H42     | 1.68                     | 0.41              |
| 4:QD:38:TYR:HB2   | 4:QD:44:GLY:O      | 2.21                     | 0.41              |
| 5:QE:12:LEU:O     | 5:QE:13:ILE:HD12   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:QG:70:LYS:HA    | 7:QG:71:PRO:HD2    | 1.89                     | 0.41              |
| 7:QG:93:PRO:O     | 7:QG:96:GLN:HB2    | 2.21                     | 0.41              |
| 19:QS:36:ARG:HA   | 19:QS:71:LEU:HB2   | 2.02                     | 0.41              |
| 51:R5:56:LYS:CE   | 51:R5:58:LEU:CD2   | 2.92                     | 0.41              |
| 1:QA:1475:G:H4'   | 25:RA:1689:A:H4'   | 2.01                     | 0.41              |
| 25:RA:210:C:H4'   | 25:RA:1367:A:H1'   | 2.02                     | 0.41              |
| 25:RA:48:G:H22    | 25:RA:177:G:H5''   | 1.84                     | 0.41              |
| 25:RA:588:U:H1'   | 29:RF:90:PHE:CG    | 2.56                     | 0.41              |
| 25:RA:862:G:H2'   | 25:RA:863:A:O4'    | 2.21                     | 0.41              |
| 25:RA:859:G:N2    | 25:RA:917:A:OP2    | 2.49                     | 0.41              |
| 25:RA:848:G:O6    | 25:RA:929:G:H2'    | 2.21                     | 0.41              |
| 27:RD:127:VAL:HA  | 27:RD:193:VAL:HG22 | 2.02                     | 0.41              |
| 25:RA:782:A:O2'   | 27:RD:225:ALA:HB1  | 2.20                     | 0.41              |
| 28:RE:20:ALA:O    | 28:RE:21:VAL:CG1   | 2.51                     | 0.41              |
| 28:RE:35:GLN:HB3  | 28:RE:48:GLN:HB2   | 2.02                     | 0.41              |
| 31:RH:33:LEU:HD11 | 31:RH:136:ILE:O    | 2.20                     | 0.41              |
| 31:RH:4:ILE:O     | 31:RH:6:ARG:N      | 2.51                     | 0.41              |
| 32:RI:14:ASP:O    | 32:RI:16:GLY:N     | 2.54                     | 0.41              |
| 33:RN:57:ALA:C    | 33:RN:60:ILE:HD11  | 2.40                     | 0.41              |
| 33:RN:57:ALA:O    | 33:RN:60:ILE:HD11  | 2.21                     | 0.41              |
| 33:RN:71:ILE:HG21 | 33:RN:84:LYS:HB3   | 2.02                     | 0.41              |
| 39:RT:91:ARG:HB2  | 39:RT:121:ILE:HG13 | 2.03                     | 0.41              |
| 1:XA:1287:A:H2'   | 1:XA:1288:A:C8     | 2.55                     | 0.41              |
| 1:XA:1372:U:H2'   | 1:XA:1373:G:O4'    | 2.21                     | 0.41              |
| 3:XC:42:LEU:HD12  | 3:XC:42:LEU:HA     | 1.87                     | 0.41              |
| 12:XL:68:ALA:HB2  | 12:XL:85:ILE:HD11  | 2.03                     | 0.41              |
| 14:XN:51:GLY:O    | 14:XN:53:LEU:N     | 2.53                     | 0.41              |
| 52:Y6:36:LEU:HD13 | 52:Y6:50:ARG:CZ    | 2.51                     | 0.41              |
| 25:YA:1093:G:H4'  | 31:YH:170:ARG:NH2  | 2.35                     | 0.41              |
| 25:YA:1364:G:N2   | 25:YA:1367:A:OP2   | 2.33                     | 0.41              |
| 25:YA:2301:C:H2'  | 25:YA:2302:G:C8    | 2.56                     | 0.41              |
| 25:YA:27:G:HO2'   | 25:YA:28:A:H8      | 1.64                     | 0.41              |
| 25:YA:273:G:H1    | 25:YA:364:C:H42    | 1.67                     | 0.41              |
| 25:YA:732:C:H2'   | 25:YA:733:G:O4'    | 2.21                     | 0.41              |
| 25:YA:76:C:H1'    | 48:Y2:62:THR:HG21  | 2.02                     | 0.41              |
| 27:YD:36:PRO:HB3  | 27:YD:61:LEU:HB3   | 2.03                     | 0.41              |
| 28:YE:41:LYS:HA   | 28:YE:41:LYS:HE2   | 2.02                     | 0.41              |
| 28:YE:64:LYS:C    | 28:YE:66:HIS:H     | 2.24                     | 0.41              |
| 28:YE:86:PRO:HB2  | 28:YE:87:GLU:H     | 1.67                     | 0.41              |
| 29:YF:68:LYS:O    | 29:YF:69:HIS:CB    | 2.68                     | 0.41              |
| 30:YG:103:LEU:O   | 30:YG:107:LEU:HG   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:YP:59:LEU:HA    | 35:YP:61:ARG:NH2  | 2.36                     | 0.41              |
| 37:YR:44:LEU:HD22  | 37:YR:48:VAL:HG23 | 2.02                     | 0.41              |
| 40:YU:8:VAL:O      | 40:YU:12:ARG:HG3  | 2.20                     | 0.41              |
| 40:YU:17:ILE:HG23  | 40:YU:39:LEU:HD12 | 2.02                     | 0.41              |
| 45:YZ:136:PHE:CD1  | 45:YZ:138:GLU:HG3 | 2.56                     | 0.41              |
| 45:YZ:5:LEU:HD22   | 45:YZ:5:LEU:HA    | 1.86                     | 0.41              |
| 1:QA:1314:C:P      | 19:QS:6:LYS:HD2   | 2.61                     | 0.41              |
| 1:QA:149:A:H4'     | 1:QA:1450:U:C4    | 2.55                     | 0.41              |
| 1:QA:618:C:H5'     | 1:QA:619:U:H5''   | 2.03                     | 0.41              |
| 8:QH:44:PHE:HD1    | 8:QH:80:ILE:HG12  | 1.86                     | 0.41              |
| 17:QQ:92:ARG:HD3   | 17:QQ:92:ARG:HA   | 1.91                     | 0.41              |
| 46:R0:12:ASN:HB3   | 46:R0:13:GLY:H    | 1.67                     | 0.41              |
| 47:R1:58:ILE:CD1   | 47:R1:86:SER:HB2  | 2.50                     | 0.41              |
| 50:R4:39:CYS:HB2   | 50:R4:41:PRO:HD2  | 2.02                     | 0.41              |
| 25:RA:1070:A:N7    | 25:RA:1096:A:H2'  | 2.36                     | 0.41              |
| 25:RA:1091:G:N2    | 25:RA:1101:U:H1'  | 2.36                     | 0.41              |
| 25:RA:2414:G:H21   | 35:RP:67:MET:CE   | 2.33                     | 0.41              |
| 25:RA:2820:A:O2'   | 25:RA:2821:A:OP1  | 2.34                     | 0.41              |
| 26:RB:13:A:H2'     | 26:RB:14:U:H5''   | 2.02                     | 0.41              |
| 25:RA:797:C:OP2    | 29:RF:62:ARG:HB2  | 2.21                     | 0.41              |
| 31:RH:125:VAL:HG13 | 31:RH:126:PRO:CG  | 2.46                     | 0.41              |
| 31:RH:152:ARG:HE   | 31:RH:153:LYS:HZ3 | 1.69                     | 0.41              |
| 32:RI:12:LEU:HG    | 32:RI:19:VAL:HG11 | 2.03                     | 0.41              |
| 34:RO:26:LYS:HB2   | 34:RO:30:ALA:HB2  | 2.02                     | 0.41              |
| 34:RO:73:ASP:OD2   | 39:RT:32:TYR:OH   | 2.28                     | 0.41              |
| 25:RA:566:U:OP1    | 35:RP:29:LYS:HE2  | 2.21                     | 0.41              |
| 1:XA:110:C:H2'     | 1:XA:111:G:O4'    | 2.21                     | 0.41              |
| 1:XA:1355:G:H2'    | 1:XA:1356:G:C8    | 2.55                     | 0.41              |
| 1:XA:186:C:H2'     | 1:XA:186(A):C:C6  | 2.56                     | 0.41              |
| 1:XA:567:G:C2      | 1:XA:568:G:H1'    | 2.56                     | 0.41              |
| 2:XB:118:LEU:CB    | 2:XB:142:LEU:HD12 | 2.50                     | 0.41              |
| 4:XD:64:LEU:HD13   | 4:XD:198:VAL:HG11 | 2.03                     | 0.41              |
| 5:XE:82:VAL:HB     | 5:XE:138:ALA:HB2  | 2.03                     | 0.41              |
| 5:XE:68:GLU:HG3    | 5:XE:68:GLU:O     | 2.21                     | 0.41              |
| 23:XW:4:C:H2'      | 23:XW:5:G:C8      | 2.55                     | 0.41              |
| 23:XW:18:G:N1      | 23:XW:55:U:H1'    | 2.36                     | 0.41              |
| 22:XV:1:G:H4'      | 46:Y0:7:LEU:O     | 2.20                     | 0.41              |
| 47:Y1:83:GLU:C     | 47:Y1:85:LEU:H    | 2.24                     | 0.41              |
| 25:YA:1344:G:H4'   | 25:YA:1384:A:C5   | 2.55                     | 0.41              |
| 25:YA:1359:A:N7    | 25:YA:1373:A:C6   | 2.89                     | 0.41              |
| 25:YA:1810:A:H8    | 25:YA:1810:A:O5'  | 2.04                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2335:A:HO2' | 25:YA:2336:A:C5'   | 2.31                     | 0.41              |
| 25:YA:774:A:H2    | 25:YA:787:U:O2'    | 2.03                     | 0.41              |
| 25:YA:814:C:H41   | 35:YP:25:SER:HA    | 1.84                     | 0.41              |
| 25:YA:848:G:O6    | 25:YA:929:G:H2'    | 2.20                     | 0.41              |
| 25:YA:968:G:H2'   | 25:YA:969:U:O4'    | 2.21                     | 0.41              |
| 27:YD:102:LYS:C   | 27:YD:103:ARG:HG2  | 2.40                     | 0.41              |
| 27:YD:130:ALA:C   | 27:YD:131:LEU:HD12 | 2.42                     | 0.41              |
| 27:YD:3:VAL:HG13  | 27:YD:17:THR:HG23  | 2.03                     | 0.41              |
| 30:YG:61:ALA:HA   | 30:YG:64:THR:HG22  | 2.02                     | 0.41              |
| 31:YH:153:LYS:HZ2 | 31:YH:153:LYS:HA   | 1.84                     | 0.41              |
| 32:YI:21:VAL:HG22 | 32:YI:22:LYS:H     | 1.85                     | 0.41              |
| 32:YI:37:VAL:HG12 | 32:YI:38:LEU:H     | 1.84                     | 0.41              |
| 33:YN:96:GLU:O    | 33:YN:100:GLU:HG3  | 2.20                     | 0.41              |
| 36:YQ:16:ARG:HB3  | 36:YQ:17:LEU:H     | 1.76                     | 0.41              |
| 36:YQ:80:GLU:HB2  | 36:YQ:81:VAL:H     | 1.69                     | 0.41              |
| 45:YZ:182:LYS:CB  | 45:YZ:183:LEU:HA   | 2.51                     | 0.41              |
| 25:RA:2611:U:C4   | 56:Z7:1:T17:H31    | 2.56                     | 0.41              |
| 1:QA:1095:U:OP1   | 1:QA:1108:G:N2     | 2.54                     | 0.41              |
| 3:QC:83:ARG:O     | 3:QC:86:VAL:HG22   | 2.21                     | 0.41              |
| 5:QE:127:ASN:HA   | 5:QE:128:PRO:HD3   | 1.89                     | 0.41              |
| 5:QE:147:ASP:O    | 5:QE:151:LEU:HG    | 2.21                     | 0.41              |
| 6:QF:30:LEU:HD23  | 6:QF:75:LEU:HD11   | 2.02                     | 0.41              |
| 11:QK:25:TYR:CZ   | 11:QK:87:THR:HB    | 2.55                     | 0.41              |
| 15:QO:2:PRO:HB2   | 15:QO:3:ILE:H      | 1.56                     | 0.41              |
| 21:QU:10:ARG:HA   | 21:QU:13:ILE:HB    | 2.01                     | 0.41              |
| 53:R7:31:LEU:HA   | 53:R7:31:LEU:HD23  | 1.86                     | 0.41              |
| 25:RA:1752:C:H42  | 25:RA:1756:G:H1    | 1.69                     | 0.41              |
| 25:RA:217:G:H2'   | 25:RA:218:A:O4'    | 2.21                     | 0.41              |
| 25:RA:2697:G:H2'  | 25:RA:2698:U:O4'   | 2.21                     | 0.41              |
| 25:RA:328:U:H4'   | 44:RY:68:HIS:CD2   | 2.56                     | 0.41              |
| 25:RA:755:C:H2'   | 25:RA:756:C:C6     | 2.56                     | 0.41              |
| 25:RA:840:C:H2'   | 25:RA:841:A:C8     | 2.56                     | 0.41              |
| 26:RB:79:C:H2'    | 26:RB:80:U:O4'     | 2.20                     | 0.41              |
| 27:RD:111:LEU:HA  | 27:RD:111:LEU:HD23 | 1.78                     | 0.41              |
| 27:RD:150:LYS:N   | 27:RD:150:LYS:HD3  | 2.36                     | 0.41              |
| 27:RD:226:MET:HB3 | 27:RD:230:ASP:HB2  | 2.03                     | 0.41              |
| 27:RD:34:VAL:C    | 27:RD:35:LYS:HG3   | 2.40                     | 0.41              |
| 28:RE:144:ARG:HB3 | 28:RE:145:LYS:H    | 1.47                     | 0.41              |
| 33:RN:73:THR:HB   | 33:RN:82:LEU:HD11  | 2.02                     | 0.41              |
| 33:RN:9:VAL:HG21  | 33:RN:48:MET:HB3   | 2.02                     | 0.41              |
| 35:RP:62:LEU:N    | 35:RP:62:LEU:HD13  | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:66:ILE:HG13  | 36:RQ:67:ARG:N     | 2.36                     | 0.41              |
| 38:RS:62:LYS:HB3   | 38:RS:97:ARG:CD    | 2.44                     | 0.41              |
| 45:RZ:74:VAL:HG22  | 45:RZ:86:VAL:HG22  | 2.03                     | 0.41              |
| 45:RZ:97:GLU:O     | 45:RZ:98:MET:HB3   | 2.21                     | 0.41              |
| 1:XA:1095:U:H2'    | 1:XA:1096:C:C6     | 2.56                     | 0.41              |
| 1:XA:946:A:H2'     | 1:XA:947:G:C8      | 2.56                     | 0.41              |
| 2:XB:166:ASP:HB3   | 2:XB:169:LYS:HB2   | 2.02                     | 0.41              |
| 3:XC:138:VAL:HG13  | 3:XC:149:ALA:HB3   | 2.02                     | 0.41              |
| 8:XH:12:ARG:HD3    | 8:XH:26:VAL:HB     | 2.03                     | 0.41              |
| 9:XI:79:LEU:O      | 9:XI:83:ARG:HG2    | 2.19                     | 0.41              |
| 9:XI:95:LYS:NZ     | 9:XI:96:LEU:HD13   | 2.36                     | 0.41              |
| 10:XJ:54:PHE:CD2   | 10:XJ:55:LYS:HG3   | 2.56                     | 0.41              |
| 20:XT:11:SER:HA    | 20:XT:13:LEU:HD12  | 2.01                     | 0.41              |
| 23:XW:8:U:H5'      | 23:XW:49:C:OP2     | 2.21                     | 0.41              |
| 50:Y4:43:TYR:O     | 50:Y4:46:GLN:HA    | 2.20                     | 0.41              |
| 50:Y4:55:ARG:O     | 50:Y4:55:ARG:HG2   | 2.21                     | 0.41              |
| 54:Y8:37:SER:O     | 54:Y8:40:GLU:HB3   | 2.21                     | 0.41              |
| 25:YA:1007:C:OP1   | 33:YN:35:ARG:NH1   | 2.52                     | 0.41              |
| 25:YA:1026:U:H4'   | 25:YA:1027:A:OP1   | 2.21                     | 0.41              |
| 25:YA:1029:A:O5'   | 25:YA:1029:A:H8    | 2.04                     | 0.41              |
| 25:YA:1385:G:H1'   | 25:YA:1386:C:C6    | 2.56                     | 0.41              |
| 25:YA:1657:C:H2'   | 25:YA:1658:C:C6    | 2.55                     | 0.41              |
| 25:YA:83:G:H21     | 25:YA:103:A:H62    | 1.69                     | 0.41              |
| 27:YD:145:VAL:HG11 | 27:YD:175:LEU:HD11 | 2.02                     | 0.41              |
| 27:YD:35:LYS:HZ1   | 27:YD:65:ILE:HA    | 1.85                     | 0.41              |
| 30:YG:124:SER:HB2  | 30:YG:131:TYR:CE1  | 2.56                     | 0.41              |
| 30:YG:18:GLU:OE1   | 30:YG:22:ARG:NH1   | 2.49                     | 0.41              |
| 40:YU:92:ARG:HD2   | 40:YU:95:LEU:HD12  | 2.02                     | 0.41              |
| 40:YU:92:ARG:NH2   | 41:YV:11:GLN:H     | 2.18                     | 0.41              |
| 43:YX:31:HIS:HB3   | 43:YX:34:ALA:HB2   | 2.03                     | 0.41              |
| 45:YZ:8:TYR:HD2    | 45:YZ:38:TYR:CZ    | 2.39                     | 0.41              |
| 1:QA:1035:A:N6     | 1:QA:1036:G:N3     | 2.69                     | 0.41              |
| 1:QA:1143:G:H2'    | 1:QA:1144:G:C8     | 2.55                     | 0.41              |
| 1:QA:34:C:H2'      | 1:QA:35:G:H8       | 1.86                     | 0.41              |
| 4:QD:63:LYS:HE3    | 4:QD:63:LYS:HB2    | 1.77                     | 0.41              |
| 7:QG:150:ALA:O     | 11:QK:57:THR:CG2   | 2.69                     | 0.41              |
| 8:QH:41:ARG:NH2    | 8:QH:123:GLU:OE2   | 2.54                     | 0.41              |
| 15:QO:32:LEU:HA    | 15:QO:32:LEU:HD23  | 1.76                     | 0.41              |
| 50:R4:23:GLU:HG3   | 50:R4:25:TYR:HE2   | 1.85                     | 0.41              |
| 52:R6:24:GLU:HB3   | 52:R6:25:LYS:H     | 1.74                     | 0.41              |
| 25:RA:1179:C:H2'   | 25:RA:1180:C:O4'   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2168:G:OP2   | 25:RA:2168:G:H8    | 2.04                     | 0.41              |
| 25:RA:2422:A:N7    | 54:R8:31:HIS:NE2   | 2.56                     | 0.41              |
| 25:RA:242:G:H4'    | 25:RA:243:U:O5'    | 2.21                     | 0.41              |
| 25:RA:2692:C:H2'   | 25:RA:2693:A:C8    | 2.55                     | 0.41              |
| 25:RA:700:G:H2'    | 25:RA:701:G:O4'    | 2.21                     | 0.41              |
| 29:RF:33:LEU:HD12  | 29:RF:33:LEU:HA    | 1.83                     | 0.41              |
| 30:RG:131:TYR:O    | 30:RG:159:VAL:HG13 | 2.21                     | 0.41              |
| 31:RH:107:VAL:HB   | 31:RH:153:LYS:HE3  | 2.03                     | 0.41              |
| 32:RI:120:ILE:HD11 | 32:RI:126:TYR:OH   | 2.20                     | 0.41              |
| 37:RR:70:LEU:C     | 37:RR:72:ASP:H     | 2.21                     | 0.41              |
| 38:RS:83:LYS:C     | 38:RS:109:GLY:HA3  | 2.42                     | 0.41              |
| 40:RU:83:LEU:HG    | 40:RU:88:ILE:HB    | 2.03                     | 0.41              |
| 43:RX:67:GLY:C     | 43:RX:69:TYR:H     | 2.23                     | 0.41              |
| 45:RZ:110:GLY:CA   | 45:RZ:111:VAL:C    | 2.87                     | 0.41              |
| 1:XA:1073:U:H2'    | 1:XA:1074:G:C8     | 2.56                     | 0.41              |
| 10:XJ:76:ASN:HA    | 10:XJ:77:PRO:HD2   | 1.96                     | 0.41              |
| 11:XK:38:ASN:HA    | 11:XK:39:PRO:HD3   | 1.75                     | 0.41              |
| 50:Y4:48:ARG:HH12  | 50:Y4:52:THR:H     | 1.68                     | 0.41              |
| 25:YA:1061:U:H4'   | 25:YA:1070:A:H1'   | 2.01                     | 0.41              |
| 25:YA:1578:U:C2'   | 25:YA:1579:A:H5'   | 2.51                     | 0.41              |
| 25:YA:2098:U:O2    | 25:YA:2191:G:N2    | 2.45                     | 0.41              |
| 25:YA:2185:C:H2'   | 25:YA:2186:G:C8    | 2.56                     | 0.41              |
| 25:YA:2712:U:O2'   | 25:YA:2712(A):A:P  | 2.79                     | 0.41              |
| 25:YA:2867:G:HO2'  | 25:YA:2868:A:H8    | 1.65                     | 0.41              |
| 25:YA:596:G:H2'    | 25:YA:597:U:O4'    | 2.21                     | 0.41              |
| 27:YD:201:HIS:O    | 27:YD:204:ILE:HG12 | 2.21                     | 0.41              |
| 27:YD:62:TYR:HA    | 27:YD:87:ASN:OD1   | 2.21                     | 0.41              |
| 28:YE:32:PRO:HA    | 28:YE:90:THR:HA    | 2.03                     | 0.41              |
| 29:YF:67:GLN:HG3   | 29:YF:67:GLN:O     | 2.21                     | 0.41              |
| 30:YG:7:LEU:HD12   | 30:YG:104:GLU:HA   | 2.03                     | 0.41              |
| 31:YH:125:VAL:HG22 | 31:YH:131:VAL:HG13 | 2.02                     | 0.41              |
| 31:YH:152:ARG:NE   | 31:YH:153:LYS:NZ   | 2.68                     | 0.41              |
| 32:YI:115:ALA:HB3  | 32:YI:128:LEU:HD12 | 2.02                     | 0.41              |
| 33:YN:7:LYS:H      | 33:YN:7:LYS:NZ     | 2.18                     | 0.41              |
| 35:YP:106:LEU:O    | 35:YP:107:LYS:HB2  | 2.20                     | 0.41              |
| 56:Z8:3:GLY:HA3    | 56:Z8:4:PRO:HA     | 1.77                     | 0.41              |
| 1:QA:1098:C:H2'    | 1:QA:1099:G:O4'    | 2.20                     | 0.40              |
| 1:QA:1122:U:H3     | 1:QA:1151:A:H2     | 1.66                     | 0.40              |
| 1:QA:1199:U:H4'    | 10:QJ:54:PHE:CZ    | 2.56                     | 0.40              |
| 1:QA:452:A:HO2'    | 1:QA:453:A:C4'     | 2.33                     | 0.40              |
| 1:QA:452:A:H2'     | 1:QA:453:A:C8      | 2.56                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:QA:754:C:H1'     | 15:QO:69:TYR:CD2    | 2.57                     | 0.40              |
| 1:QA:977:A:O2'     | 1:QA:979:C:OP2      | 2.31                     | 0.40              |
| 1:QA:985:C:H2'     | 1:QA:986:A:H8       | 1.84                     | 0.40              |
| 1:QA:922:G:H4'     | 5:QE:20:GLN:HA      | 2.03                     | 0.40              |
| 7:QG:54:THR:O      | 7:QG:56:GLN:N       | 2.52                     | 0.40              |
| 8:QH:83:ILE:HB     | 8:QH:137:VAL:HG13   | 2.03                     | 0.40              |
| 12:QL:27:LEU:HG    | 12:QL:62:SER:HB3    | 2.02                     | 0.40              |
| 19:QS:5:LEU:HD12   | 19:QS:5:LEU:HA      | 1.93                     | 0.40              |
| 23:QW:61:C:H2'     | 23:QW:62:C:C6       | 2.56                     | 0.40              |
| 46:R0:72:ARG:HB2   | 46:R0:75:LEU:HB2    | 2.03                     | 0.40              |
| 50:R4:13:ARG:O     | 50:R4:30:GLU:HA     | 2.21                     | 0.40              |
| 25:RA:1024:G:C6    | 25:RA:1025:G:C6     | 3.09                     | 0.40              |
| 25:RA:1676:A:H2'   | 25:RA:1677:A:O4'    | 2.21                     | 0.40              |
| 25:RA:2315:G:H2'   | 25:RA:2316:C:C6     | 2.56                     | 0.40              |
| 25:RA:2322:A:H2'   | 25:RA:2323:G:O4'    | 2.21                     | 0.40              |
| 25:RA:2845:G:O2'   | 25:RA:2846:G:H5'    | 2.21                     | 0.40              |
| 25:RA:2032:G:H1'   | 28:RE:145:LYS:HD3   | 2.03                     | 0.40              |
| 28:RE:184:VAL:HB   | 28:RE:185:LYS:H     | 1.64                     | 0.40              |
| 29:RF:107:LYS:HE3  | 29:RF:206:ILE:HD12  | 2.03                     | 0.40              |
| 30:RG:117:PHE:HE1  | 30:RG:120:LEU:HD23  | 1.86                     | 0.40              |
| 34:RO:63:VAL:HB    | 34:RO:106:LEU:HD11  | 2.02                     | 0.40              |
| 39:RT:109:GLU:O    | 39:RT:113:LYS:HB2   | 2.21                     | 0.40              |
| 39:RT:51:ARG:CG    | 39:RT:98:LYS:HG3    | 2.51                     | 0.40              |
| 1:XA:1162:C:H2'    | 1:XA:1163:C:C6      | 2.57                     | 0.40              |
| 1:XA:1053:G:C6     | 1:XA:1199:U:C2      | 3.09                     | 0.40              |
| 1:XA:1491:G:N7     | 58:XA:1672:PAR:O53  | 2.41                     | 0.40              |
| 58:XA:1672:PAR:H34 | 58:XA:1672:PAR:H642 | 1.92                     | 0.40              |
| 1:XA:235:C:H2'     | 1:XA:236:G:C8       | 2.54                     | 0.40              |
| 1:XA:312:C:H2'     | 1:XA:313:A:H8       | 1.86                     | 0.40              |
| 1:XA:537:G:H2'     | 1:XA:538:G:C8       | 2.56                     | 0.40              |
| 1:XA:672:U:H2'     | 1:XA:673:G:H8       | 1.85                     | 0.40              |
| 1:XA:730:G:C5      | 1:XA:731:G:H1'      | 2.56                     | 0.40              |
| 1:XA:78:G:O2'      | 1:XA:79:G:OP1       | 2.31                     | 0.40              |
| 1:XA:833:U:H2'     | 1:XA:834:C:C6       | 2.56                     | 0.40              |
| 2:XB:126:GLU:O     | 2:XB:129:GLU:HB2    | 2.20                     | 0.40              |
| 8:XH:6:ILE:HB      | 8:XH:85:ARG:NH1     | 2.36                     | 0.40              |
| 10:XJ:6:ILE:O      | 10:XJ:71:LEU:HD12   | 2.21                     | 0.40              |
| 11:XK:19:ALA:CB    | 11:XK:32:ILE:HG22   | 2.51                     | 0.40              |
| 1:XA:1228:C:P      | 13:XM:108:ARG:HH22  | 2.44                     | 0.40              |
| 52:Y6:11:LEU:HD13  | 52:Y6:11:LEU:HA     | 1.86                     | 0.40              |
| 25:YA:1341:U:O4'   | 43:YX:57:LEU:HD23   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1520:U:H2'   | 25:YA:1521:G:O4'  | 2.21                     | 0.40              |
| 25:YA:1651:G:N7    | 37:YR:11:ASN:ND2  | 2.60                     | 0.40              |
| 25:YA:218:A:C2     | 25:YA:235:U:H4'   | 2.57                     | 0.40              |
| 25:YA:2803:C:H2'   | 25:YA:2804:C:C6   | 2.56                     | 0.40              |
| 25:YA:2867:G:O2'   | 25:YA:2868:A:H8   | 2.03                     | 0.40              |
| 25:YA:324:A:H2'    | 25:YA:325:G:O4'   | 2.21                     | 0.40              |
| 25:YA:796:C:H2'    | 25:YA:797:C:C6    | 2.56                     | 0.40              |
| 25:YA:874:G:H2'    | 25:YA:875:G:C8    | 2.56                     | 0.40              |
| 4:QD:166:LYS:HB3   | 27:YD:134:ARG:NH1 | 2.35                     | 0.40              |
| 28:YE:95:ILE:H     | 28:YE:95:ILE:CD1  | 2.31                     | 0.40              |
| 32:YI:23:PRO:O     | 32:YI:27:ARG:HG2  | 2.21                     | 0.40              |
| 34:YO:4:PRO:O      | 34:YO:5:GLN:CB    | 2.69                     | 0.40              |
| 35:YP:29:LYS:HB3   | 35:YP:30:THR:H    | 1.59                     | 0.40              |
| 40:YU:96:ALA:HA    | 40:YU:98:LEU:HD23 | 2.03                     | 0.40              |
| 45:YZ:28:MET:O     | 45:YZ:34:ASN:HA   | 2.22                     | 0.40              |
| 1:QA:109:A:C6      | 1:QA:326:G:C6     | 3.09                     | 0.40              |
| 1:QA:10:A:H2'      | 1:QA:11:G:H8      | 1.86                     | 0.40              |
| 1:QA:271:C:H2'     | 1:QA:272:C:C6     | 2.56                     | 0.40              |
| 1:QA:509:A:O2'     | 1:QA:510:A:OP1    | 2.35                     | 0.40              |
| 1:QA:664:G:N2      | 1:QA:741:G:H1     | 2.15                     | 0.40              |
| 6:QF:35:ALA:HA     | 6:QF:67:MET:HB3   | 2.02                     | 0.40              |
| 6:QF:79:LEU:HD23   | 6:QF:79:LEU:HA    | 1.93                     | 0.40              |
| 1:QA:1367:C:H5'    | 10:QJ:60:ARG:CZ   | 2.51                     | 0.40              |
| 10:QJ:31:GLY:HA3   | 10:QJ:78:ASN:CG   | 2.41                     | 0.40              |
| 25:RA:1614:A:H62   | 42:RW:93:ALA:HB2  | 1.85                     | 0.40              |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:CZ  | 2.50                     | 0.40              |
| 28:RE:55:ASN:HD22  | 28:RE:58:ARG:HB2  | 1.87                     | 0.40              |
| 31:RH:98:LEU:HB2   | 31:RH:125:VAL:HB  | 2.03                     | 0.40              |
| 32:RI:30:LEU:HD22  | 32:RI:35:LEU:HD11 | 2.02                     | 0.40              |
| 35:RP:114:ILE:HD11 | 35:RP:130:PHE:CD2 | 2.57                     | 0.40              |
| 36:RQ:58:PHE:CD1   | 36:RQ:61:GLY:HA3  | 2.56                     | 0.40              |
| 25:RA:1649:G:O2'   | 37:RR:107:ASP:OD2 | 2.32                     | 0.40              |
| 25:RA:2685:G:P     | 39:RT:51:ARG:HH22 | 2.44                     | 0.40              |
| 45:RZ:48:PHE:HE1   | 45:RZ:71:VAL:HG21 | 1.87                     | 0.40              |
| 2:XB:120:ALA:C     | 2:XB:122:PHE:H    | 2.24                     | 0.40              |
| 2:XB:19:HIS:NE2    | 2:XB:206:ASP:HB2  | 2.36                     | 0.40              |
| 52:Y6:13:CYS:HB2   | 52:Y6:22:ALA:HB3  | 2.03                     | 0.40              |
| 25:YA:1826:G:H4'   | 27:YD:242:ARG:NH2 | 2.36                     | 0.40              |
| 25:YA:1869:G:H5'   | 25:YA:1870:C:OP2  | 2.20                     | 0.40              |
| 25:YA:2334:G:H4'   | 25:YA:2335:A:OP2  | 2.21                     | 0.40              |
| 25:YA:2633:G:H2'   | 25:YA:2634:G:O4'  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:271:G:H2'   | 25:YA:272:G:H8     | 1.86                     | 0.40              |
| 25:YA:196:A:O2'   | 25:YA:805:G:O6     | 2.34                     | 0.40              |
| 25:YA:1843:C:H5'  | 27:YD:253:GLN:OE1  | 2.21                     | 0.40              |
| 25:YA:1797:C:H4'  | 27:YD:257:LEU:O    | 2.21                     | 0.40              |
| 29:YF:28:ILE:H    | 29:YF:28:ILE:HG13  | 1.68                     | 0.40              |
| 31:YH:15:VAL:HG21 | 31:YH:76:VAL:CG1   | 2.44                     | 0.40              |
| 1:QA:1325:C:OP2   | 21:QU:6:ARG:NH2    | 2.49                     | 0.40              |
| 1:QA:337:C:H2'    | 1:QA:338:A:C8      | 2.57                     | 0.40              |
| 6:QF:33:TYR:CE1   | 6:QF:78:GLU:HG2    | 2.56                     | 0.40              |
| 10:QJ:4:ILE:HA    | 10:QJ:100:THR:HG22 | 2.02                     | 0.40              |
| 51:R5:58:LEU:CD1  | 51:R5:58:LEU:H     | 2.22                     | 0.40              |
| 35:RP:62:LEU:O    | 54:R8:13:ARG:HB2   | 2.22                     | 0.40              |
| 54:R8:49:VAL:HG23 | 54:R8:53:PRO:HB3   | 2.04                     | 0.40              |
| 25:RA:1430:C:H2'  | 25:RA:1431:U:C6    | 2.57                     | 0.40              |
| 25:RA:2262:U:H2'  | 25:RA:2263:C:C6    | 2.56                     | 0.40              |
| 25:RA:303:U:H2'   | 25:RA:304:G:C8     | 2.56                     | 0.40              |
| 25:RA:341:G:H2'   | 25:RA:342:G:O4'    | 2.21                     | 0.40              |
| 25:RA:722:A:H3'   | 25:RA:723:G:H8     | 1.87                     | 0.40              |
| 25:RA:960:A:H5''  | 25:RA:961:C:OP1    | 2.22                     | 0.40              |
| 27:RD:26:LYS:HD2  | 27:RD:26:LYS:H     | 1.87                     | 0.40              |
| 31:RH:103:LEU:HG  | 31:RH:105:LEU:HD12 | 2.02                     | 0.40              |
| 38:RS:23:ARG:HB2  | 38:RS:86:ALA:HB2   | 2.03                     | 0.40              |
| 45:RZ:92:SER:HB3  | 45:RZ:93:ASP:H     | 1.66                     | 0.40              |
| 1:XA:401:C:H2'    | 1:XA:402:G:C8      | 2.56                     | 0.40              |
| 1:XA:514:C:H2'    | 1:XA:515:G:H8      | 1.87                     | 0.40              |
| 1:XA:625:G:H4'    | 16:XP:16:HIS:CD2   | 2.56                     | 0.40              |
| 1:XA:986:A:H2'    | 1:XA:987:G:O4'     | 2.21                     | 0.40              |
| 4:XD:186:LEU:HD23 | 4:XD:186:LEU:HA    | 1.95                     | 0.40              |
| 5:XE:51:VAL:HB    | 5:XE:52:PRO:HD3    | 2.04                     | 0.40              |
| 10:XJ:77:PRO:O    | 10:XJ:79:ARG:NH1   | 2.54                     | 0.40              |
| 12:XL:90:VAL:O    | 12:XL:92:ASP:N     | 2.54                     | 0.40              |
| 1:XA:376:G:OP1    | 16:XP:5:ARG:HB2    | 2.21                     | 0.40              |
| 16:XP:60:LEU:HD23 | 16:XP:60:LEU:HA    | 1.80                     | 0.40              |
| 19:XS:36:ARG:HA   | 19:XS:71:LEU:HB2   | 2.03                     | 0.40              |
| 22:XV:14:G:N2     | 22:XV:48:C:H42     | 2.19                     | 0.40              |
| 50:Y4:14:ILE:HG23 | 50:Y4:14:ILE:O     | 2.21                     | 0.40              |
| 25:YA:1688:U:O2   | 25:YA:1700:A:H5''  | 2.21                     | 0.40              |
| 25:YA:1754:C:H2'  | 25:YA:1755:A:O4'   | 2.21                     | 0.40              |
| 25:YA:1930:G:H2'  | 25:YA:1968:G:N1    | 2.36                     | 0.40              |
| 25:YA:357:A:H2'   | 25:YA:358:U:C6     | 2.57                     | 0.40              |
| 28:YE:49:LEU:HD12 | 28:YE:49:LEU:HA    | 1.72                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:YF:64:ILE:HA    | 29:YF:64:ILE:HD12 | 1.80                     | 0.40              |
| 32:YI:38:LEU:HD12  | 32:YI:38:LEU:H    | 1.86                     | 0.40              |
| 33:YN:65:LYS:HG2   | 33:YN:65:LYS:H    | 1.60                     | 0.40              |
| 38:YS:69:VAL:HA    | 38:YS:72:ALA:HB3  | 2.03                     | 0.40              |
| 40:YU:19:LYS:O     | 40:YU:22:LYS:HB2  | 2.21                     | 0.40              |
| 45:YZ:96:VAL:CG1   | 45:YZ:128:VAL:O   | 2.66                     | 0.40              |
| 1:QA:1300:G:N1     | 1:QA:1335:C:O4'   | 2.55                     | 0.40              |
| 1:QA:976:G:N2      | 1:QA:1362:C:H2'   | 2.36                     | 0.40              |
| 1:QA:298:A:H2'     | 1:QA:299:G:O4'    | 2.22                     | 0.40              |
| 1:QA:422:C:O2'     | 1:QA:423:G:H5''   | 2.22                     | 0.40              |
| 1:QA:766:A:H2'     | 1:QA:767:A:O4'    | 2.21                     | 0.40              |
| 1:QA:985:C:H2'     | 1:QA:986:A:C8     | 2.57                     | 0.40              |
| 3:QC:71:ALA:HB2    | 3:QC:109:PRO:HB3  | 2.04                     | 0.40              |
| 4:QD:176:LEU:HD12  | 4:QD:182:LYS:O    | 2.21                     | 0.40              |
| 8:QH:91:ARG:CB     | 12:QL:7:ILE:HG13  | 2.44                     | 0.40              |
| 13:QM:40:ASN:HA    | 13:QM:41:PRO:HD3  | 1.89                     | 0.40              |
| 13:QM:4:ILE:H      | 13:QM:9:ILE:CG2   | 2.35                     | 0.40              |
| 10:QJ:61:GLU:OE1   | 14:QN:58:LYS:HE2  | 2.21                     | 0.40              |
| 23:QW:16:U:H3'     | 23:QW:17:C:C5'    | 2.51                     | 0.40              |
| 47:R1:87:PRO:O     | 47:R1:91:LYS:HB2  | 2.21                     | 0.40              |
| 47:R1:95:LEU:HA    | 47:R1:95:LEU:HD23 | 1.94                     | 0.40              |
| 25:RA:516:C:OP1    | 51:R5:13:LYS:NZ   | 2.54                     | 0.40              |
| 25:RA:1011:G:C2    | 25:RA:1013:C:C2   | 3.10                     | 0.40              |
| 25:RA:1061:U:H3'   | 25:RA:1062:G:H5'' | 2.02                     | 0.40              |
| 25:RA:1174:A:N3    | 25:RA:1174:A:H2'  | 2.35                     | 0.40              |
| 25:RA:121:G:H4'    | 25:RA:149:A:H5'   | 2.03                     | 0.40              |
| 25:RA:1312:U:H1'   | 25:RA:1313:U:OP2  | 2.22                     | 0.40              |
| 25:RA:2605:U:H2'   | 25:RA:2606:C:C6   | 2.56                     | 0.40              |
| 25:RA:631:A:N3     | 25:RA:2415:G:O2'  | 2.47                     | 0.40              |
| 26:RB:38:C:O2      | 26:RB:48:A:H1'    | 2.22                     | 0.40              |
| 27:RD:96:HIS:CD2   | 27:RD:102:LYS:HG2 | 2.56                     | 0.40              |
| 27:RD:35:LYS:HB3   | 27:RD:63:ARG:HA   | 2.04                     | 0.40              |
| 28:RE:26:ILE:O     | 28:RE:26:ILE:HG12 | 2.18                     | 0.40              |
| 28:RE:36:ARG:HB3   | 28:RE:36:ARG:HH11 | 1.87                     | 0.40              |
| 29:RF:116:ASP:OD2  | 35:RP:1:MET:N     | 2.54                     | 0.40              |
| 29:RF:181:LEU:HD22 | 29:RF:181:LEU:HA  | 1.79                     | 0.40              |
| 29:RF:29:ASN:HB3   | 29:RF:32:LEU:HD23 | 2.04                     | 0.40              |
| 31:RH:30:LYS:HD2   | 31:RH:81:GLU:H    | 1.86                     | 0.40              |
| 32:RI:138:ILE:HG12 | 32:RI:139:GLN:N   | 2.37                     | 0.40              |
| 33:RN:108:PRO:O    | 33:RN:113:GLY:HA3 | 2.21                     | 0.40              |
| 36:RQ:72:LYS:HB3   | 36:RQ:94:VAL:O    | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:RT:120:ARG:HA   | 39:RT:123:GLN:NE2  | 2.37                     | 0.40              |
| 44:RY:11:ASP:O     | 44:RY:26:LYS:HG3   | 2.21                     | 0.40              |
| 44:RY:64:GLU:H     | 44:RY:64:GLU:HG2   | 1.64                     | 0.40              |
| 1:XA:1347:G:H22    | 1:XA:1374:A:P      | 2.43                     | 0.40              |
| 1:XA:1523:G:OP1    | 11:XK:123:LYS:NZ   | 2.42                     | 0.40              |
| 4:XD:165:MET:O     | 4:XD:167:GLY:N     | 2.54                     | 0.40              |
| 5:XE:34:VAL:HG11   | 5:XE:63:ARG:HG2    | 2.03                     | 0.40              |
| 5:XE:89:ILE:HG12   | 5:XE:91:LEU:CD1    | 2.52                     | 0.40              |
| 6:XF:16:GLN:HA     | 6:XF:19:LEU:HB2    | 2.03                     | 0.40              |
| 12:XL:68:ALA:HB1   | 12:XL:100:ILE:HG13 | 2.03                     | 0.40              |
| 19:XS:15:LEU:HA    | 19:XS:18:LYS:HB3   | 2.04                     | 0.40              |
| 49:Y3:12:PRO:O     | 49:Y3:14:GLY:N     | 2.55                     | 0.40              |
| 52:Y6:28:ARG:HD2   | 52:Y6:28:ARG:HA    | 1.86                     | 0.40              |
| 52:Y6:28:ARG:HB3   | 52:Y6:30:THR:C     | 2.41                     | 0.40              |
| 25:YA:1186:G:H2'   | 25:YA:1187:G:O4'   | 2.20                     | 0.40              |
| 25:YA:1329:U:H5''  | 25:YA:1330:C:H5    | 1.86                     | 0.40              |
| 25:YA:2010:G:H5''  | 42:YW:42:ARG:HB2   | 2.03                     | 0.40              |
| 25:YA:2579:C:H2'   | 25:YA:2580:U:O4'   | 2.21                     | 0.40              |
| 25:YA:2776:A:OP1   | 25:YA:2776:A:H3'   | 2.21                     | 0.40              |
| 25:YA:900:A:H3'    | 25:YA:901:A:C8     | 2.54                     | 0.40              |
| 29:YF:168:ARG:HG3  | 29:YF:175:THR:HG21 | 2.02                     | 0.40              |
| 29:YF:125:LEU:HD21 | 29:YF:199:TRP:CE3  | 2.57                     | 0.40              |
| 31:YH:46:GLU:OE1   | 31:YH:51:ARG:NH1   | 2.54                     | 0.40              |
| 40:YU:61:TRP:O     | 40:YU:65:ILE:HG13  | 2.22                     | 0.40              |
| 41:YV:21:ARG:HD2   | 41:YV:91:TYR:CE1   | 2.56                     | 0.40              |
| 44:YY:89:PHE:C     | 44:YY:90:LEU:HD13  | 2.42                     | 0.40              |
| 1:QA:1469:G:H2'    | 1:QA:1470:G:C8     | 2.57                     | 0.40              |
| 1:QA:148:G:H2'     | 1:QA:149:A:C8      | 2.55                     | 0.40              |
| 1:QA:181:G:HO2'    | 1:QA:182:U:P       | 2.45                     | 0.40              |
| 1:QA:410:G:H4'     | 1:QA:411:A:OP1     | 2.21                     | 0.40              |
| 1:QA:486:U:H2'     | 1:QA:487:A:H8      | 1.87                     | 0.40              |
| 3:QC:7:PRO:O       | 3:QC:11:ARG:NH1    | 2.54                     | 0.40              |
| 4:QD:195:ALA:O     | 6:XF:16:GLN:HB3    | 2.22                     | 0.40              |
| 4:QD:46:LYS:HD3    | 4:QD:46:LYS:HA     | 1.78                     | 0.40              |
| 5:QE:50:GLU:HG3    | 5:QE:52:PRO:HD2    | 2.04                     | 0.40              |
| 6:QF:21:LEU:O      | 6:QF:25:ILE:HG12   | 2.20                     | 0.40              |
| 1:QA:376:G:H5''    | 16:QP:5:ARG:HB2    | 2.02                     | 0.40              |
| 46:R0:68:GLU:HG2   | 46:R0:80:HIS:HB2   | 2.04                     | 0.40              |
| 25:RA:379:G:N2     | 47:R1:42:GLN:OE1   | 2.48                     | 0.40              |
| 51:R5:46:CYS:HA    | 51:R5:47:PRO:HD2   | 1.86                     | 0.40              |
| 25:RA:2123:G:H2'   | 25:RA:2124:G:C8    | 2.54                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2308:G:C2   | 25:RA:2311:A:H2    | 2.37                     | 0.40              |
| 25:RA:380:U:H2'   | 25:RA:381:G:C8     | 2.56                     | 0.40              |
| 25:RA:71:A:H5''   | 25:RA:72:U:O5'     | 2.21                     | 0.40              |
| 25:RA:196:A:O2'   | 25:RA:805:G:O6     | 2.32                     | 0.40              |
| 25:RA:955:C:OP2   | 36:RQ:14:ARG:HD2   | 2.21                     | 0.40              |
| 27:RD:209:ALA:O   | 27:RD:212:SER:HB2  | 2.22                     | 0.40              |
| 27:RD:44:ASN:HB2  | 27:RD:49:ILE:HA    | 2.02                     | 0.40              |
| 33:RN:17:ASP:O    | 33:RN:19:GLU:N     | 2.54                     | 0.40              |
| 34:RO:66:LYS:HA   | 34:RO:79:PHE:O     | 2.22                     | 0.40              |
| 35:RP:25:SER:OG   | 35:RP:26:GLY:O     | 2.38                     | 0.40              |
| 39:RT:26:ASP:CB   | 39:RT:91:ARG:HA    | 2.52                     | 0.40              |
| 40:RU:66:ASN:CG   | 40:RU:70:ARG:HH21  | 2.21                     | 0.40              |
| 45:RZ:10:ARG:HH21 | 45:RZ:26:GLY:H     | 1.69                     | 0.40              |
| 1:XA:545:C:H2'    | 1:XA:546:G:O4'     | 2.21                     | 0.40              |
| 1:XA:575:G:O2'    | 1:XA:821:G:H5'     | 2.22                     | 0.40              |
| 1:XA:611:A:H61    | 1:XA:629:G:H1      | 1.68                     | 0.40              |
| 3:XC:20:SER:HB2   | 3:XC:40:ARG:NH2    | 2.28                     | 0.40              |
| 3:XC:56:ASP:HB2   | 3:XC:67:THR:HB     | 2.03                     | 0.40              |
| 9:XI:5:TYR:HA     | 9:XI:17:VAL:O      | 2.21                     | 0.40              |
| 9:XI:75:ASP:HA    | 9:XI:78:LYS:HB3    | 2.04                     | 0.40              |
| 11:XK:18:ARG:HB3  | 11:XK:33:THR:OG1   | 2.21                     | 0.40              |
| 12:XL:18:VAL:HG23 | 12:XL:19:ARG:H     | 1.86                     | 0.40              |
| 12:XL:38:THR:CG2  | 12:XL:57:LYS:HB3   | 2.49                     | 0.40              |
| 12:XL:85:ILE:HA   | 12:XL:85:ILE:HD12  | 1.74                     | 0.40              |
| 23:XW:41:C:H2'    | 23:XW:42:C:O4'     | 2.21                     | 0.40              |
| 47:Y1:87:PRO:O    | 47:Y1:91:LYS:HB2   | 2.20                     | 0.40              |
| 49:Y3:52:HIS:CD2  | 49:Y3:53:LEU:HG    | 2.57                     | 0.40              |
| 49:Y3:5:LYS:HE3   | 49:Y3:34:GLU:OE2   | 2.22                     | 0.40              |
| 25:YA:942:G:O2'   | 25:YA:1189:A:N3    | 2.49                     | 0.40              |
| 25:YA:1417:C:H2'  | 25:YA:1418:G:O4'   | 2.21                     | 0.40              |
| 25:YA:1782:C:H1'  | 25:YA:2609:U:H5''  | 2.03                     | 0.40              |
| 25:YA:1932:A:H2'  | 25:YA:1933:G:O4'   | 2.21                     | 0.40              |
| 25:YA:2577:A:H2'  | 25:YA:2614:A:N6    | 2.36                     | 0.40              |
| 25:YA:535:C:O3'   | 40:YU:53:ARG:NH1   | 2.54                     | 0.40              |
| 25:YA:57:C:H2'    | 25:YA:58:G:O4'     | 2.21                     | 0.40              |
| 27:YD:150:LYS:HA  | 27:YD:150:LYS:HD3  | 1.94                     | 0.40              |
| 27:YD:237:GLU:O   | 27:YD:238:GLY:C    | 2.59                     | 0.40              |
| 29:YF:122:LYS:HD3 | 29:YF:122:LYS:HA   | 1.86                     | 0.40              |
| 29:YF:198:ALA:HA  | 29:YF:201:VAL:HG12 | 2.03                     | 0.40              |
| 39:YT:19:LEU:HA   | 39:YT:20:PRO:HD3   | 1.91                     | 0.40              |
| 40:YU:17:ILE:HA   | 40:YU:17:ILE:HD13  | 1.92                     | 0.40              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 41:YV:3:ALA:HA  | 41:YV:40:LEU:O     | 2.21                     | 0.40              |
| 45:YZ:136:PHE:C | 45:YZ:137:ILE:HG12 | 2.41                     | 0.40              |

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

| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 25:RA:2197:U:OP1 | 4:XD:159:ARG:NH2[4_555] | 2.05                     | 0.15              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | QB    | 235/256 (92%) | 173 (74%) | 45 (19%) | 17 (7%)  | 1           | 13  |
| 2   | XB    | 235/256 (92%) | 177 (75%) | 43 (18%) | 15 (6%)  | 1           | 17  |
| 3   | QC    | 203/239 (85%) | 163 (80%) | 34 (17%) | 6 (3%)   | 4           | 33  |
| 3   | XC    | 203/239 (85%) | 171 (84%) | 29 (14%) | 3 (2%)   | 10          | 47  |
| 4   | QD    | 206/209 (99%) | 177 (86%) | 22 (11%) | 7 (3%)   | 3           | 31  |
| 4   | XD    | 206/209 (99%) | 178 (86%) | 23 (11%) | 5 (2%)   | 6           | 37  |
| 5   | QE    | 149/162 (92%) | 136 (91%) | 8 (5%)   | 5 (3%)   | 3           | 31  |
| 5   | XE    | 149/162 (92%) | 133 (89%) | 13 (9%)  | 3 (2%)   | 7           | 41  |
| 6   | QF    | 99/101 (98%)  | 93 (94%)  | 3 (3%)   | 3 (3%)   | 4           | 33  |
| 6   | XF    | 99/101 (98%)  | 94 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 7   | QG    | 153/156 (98%) | 135 (88%) | 16 (10%) | 2 (1%)   | 12          | 50  |
| 7   | XG    | 153/156 (98%) | 138 (90%) | 13 (8%)  | 2 (1%)   | 12          | 50  |
| 8   | QH    | 136/138 (99%) | 121 (89%) | 14 (10%) | 1 (1%)   | 22          | 61  |
| 8   | XH    | 136/138 (99%) | 120 (88%) | 12 (9%)  | 4 (3%)   | 4           | 33  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | QI    | 125/128 (98%) | 103 (82%) | 17 (14%) | 5 (4%)   | 3           | 26  |
| 9   | XI    | 125/128 (98%) | 97 (78%)  | 24 (19%) | 4 (3%)   | 4           | 31  |
| 10  | QJ    | 97/105 (92%)  | 75 (77%)  | 19 (20%) | 3 (3%)   | 4           | 32  |
| 10  | XJ    | 97/105 (92%)  | 78 (80%)  | 14 (14%) | 5 (5%)   | 2           | 20  |
| 11  | QK    | 117/129 (91%) | 100 (86%) | 14 (12%) | 3 (3%)   | 5           | 35  |
| 11  | XK    | 117/129 (91%) | 100 (86%) | 15 (13%) | 2 (2%)   | 9           | 45  |
| 12  | QL    | 123/132 (93%) | 98 (80%)  | 18 (15%) | 7 (6%)   | 1           | 18  |
| 12  | XL    | 123/132 (93%) | 97 (79%)  | 14 (11%) | 12 (10%) | 0           | 8   |
| 13  | QM    | 119/126 (94%) | 95 (80%)  | 15 (13%) | 9 (8%)   | 1           | 12  |
| 13  | XM    | 119/126 (94%) | 94 (79%)  | 15 (13%) | 10 (8%)  | 1           | 10  |
| 14  | QN    | 58/61 (95%)   | 49 (84%)  | 5 (9%)   | 4 (7%)   | 1           | 14  |
| 14  | XN    | 58/61 (95%)   | 46 (79%)  | 6 (10%)  | 6 (10%)  | 0           | 7   |
| 15  | QO    | 86/89 (97%)   | 80 (93%)  | 5 (6%)   | 1 (1%)   | 13          | 51  |
| 15  | XO    | 86/89 (97%)   | 80 (93%)  | 4 (5%)   | 2 (2%)   | 6           | 38  |
| 16  | QP    | 82/88 (93%)   | 73 (89%)  | 8 (10%)  | 1 (1%)   | 13          | 51  |
| 16  | XP    | 82/88 (93%)   | 71 (87%)  | 10 (12%) | 1 (1%)   | 13          | 51  |
| 17  | QQ    | 98/105 (93%)  | 91 (93%)  | 5 (5%)   | 2 (2%)   | 7           | 41  |
| 17  | XQ    | 98/105 (93%)  | 88 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 18  | QR    | 68/88 (77%)   | 56 (82%)  | 9 (13%)  | 3 (4%)   | 2           | 23  |
| 18  | XR    | 68/88 (77%)   | 61 (90%)  | 6 (9%)   | 1 (2%)   | 10          | 47  |
| 19  | QS    | 82/93 (88%)   | 55 (67%)  | 16 (20%) | 11 (13%) | 0           | 4   |
| 19  | XS    | 82/93 (88%)   | 54 (66%)  | 17 (21%) | 11 (13%) | 0           | 4   |
| 20  | QT    | 97/106 (92%)  | 76 (78%)  | 15 (16%) | 6 (6%)   | 1           | 17  |
| 20  | XT    | 97/106 (92%)  | 75 (77%)  | 16 (16%) | 6 (6%)   | 1           | 17  |
| 21  | QU    | 23/27 (85%)   | 19 (83%)  | 3 (13%)  | 1 (4%)   | 2           | 24  |
| 21  | XU    | 23/27 (85%)   | 18 (78%)  | 4 (17%)  | 1 (4%)   | 2           | 24  |
| 27  | RD    | 270/276 (98%) | 226 (84%) | 32 (12%) | 12 (4%)  | 2           | 23  |
| 27  | YD    | 270/276 (98%) | 228 (84%) | 33 (12%) | 9 (3%)   | 4           | 31  |
| 28  | RE    | 203/206 (98%) | 148 (73%) | 35 (17%) | 20 (10%) | 0           | 8   |
| 28  | YE    | 203/206 (98%) | 144 (71%) | 42 (21%) | 17 (8%)  | 1           | 10  |
| 29  | RF    | 200/210 (95%) | 170 (85%) | 18 (9%)  | 12 (6%)  | 1           | 17  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 29  | YF    | 200/210 (95%) | 168 (84%) | 24 (12%) | 8 (4%)   | 3           | 26 |
| 30  | RG    | 179/182 (98%) | 139 (78%) | 26 (14%) | 14 (8%)  | 1           | 11 |
| 30  | YG    | 179/182 (98%) | 142 (79%) | 25 (14%) | 12 (7%)  | 1           | 15 |
| 31  | RH    | 168/180 (93%) | 116 (69%) | 33 (20%) | 19 (11%) | 0           | 6  |
| 31  | YH    | 168/180 (93%) | 124 (74%) | 23 (14%) | 21 (12%) | 0           | 5  |
| 32  | RI    | 144/148 (97%) | 104 (72%) | 27 (19%) | 13 (9%)  | 1           | 9  |
| 32  | YI    | 144/148 (97%) | 107 (74%) | 20 (14%) | 17 (12%) | 0           | 5  |
| 33  | RN    | 136/140 (97%) | 104 (76%) | 20 (15%) | 12 (9%)  | 1           | 9  |
| 33  | YN    | 136/140 (97%) | 105 (77%) | 17 (12%) | 14 (10%) | 0           | 7  |
| 34  | RO    | 120/122 (98%) | 109 (91%) | 9 (8%)   | 2 (2%)   | 9           | 45 |
| 34  | YO    | 120/122 (98%) | 108 (90%) | 10 (8%)  | 2 (2%)   | 9           | 45 |
| 35  | RP    | 148/150 (99%) | 106 (72%) | 28 (19%) | 14 (10%) | 0           | 8  |
| 35  | YP    | 148/150 (99%) | 108 (73%) | 22 (15%) | 18 (12%) | 0           | 5  |
| 36  | RQ    | 139/141 (99%) | 99 (71%)  | 22 (16%) | 18 (13%) | 0           | 5  |
| 36  | YQ    | 139/141 (99%) | 98 (70%)  | 22 (16%) | 19 (14%) | 0           | 4  |
| 37  | RR    | 116/118 (98%) | 106 (91%) | 5 (4%)   | 5 (4%)   | 2           | 24 |
| 37  | YR    | 116/118 (98%) | 99 (85%)  | 11 (10%) | 6 (5%)   | 2           | 20 |
| 38  | RS    | 109/112 (97%) | 76 (70%)  | 22 (20%) | 11 (10%) | 0           | 7  |
| 38  | YS    | 109/112 (97%) | 79 (72%)  | 17 (16%) | 13 (12%) | 0           | 5  |
| 39  | RT    | 135/146 (92%) | 107 (79%) | 16 (12%) | 12 (9%)  | 1           | 9  |
| 39  | YT    | 135/146 (92%) | 108 (80%) | 17 (13%) | 10 (7%)  | 1           | 13 |
| 40  | RU    | 115/118 (98%) | 102 (89%) | 9 (8%)   | 4 (4%)   | 3           | 30 |
| 40  | YU    | 115/118 (98%) | 102 (89%) | 9 (8%)   | 4 (4%)   | 3           | 30 |
| 41  | RV    | 99/101 (98%)  | 82 (83%)  | 11 (11%) | 6 (6%)   | 1           | 17 |
| 41  | YV    | 99/101 (98%)  | 79 (80%)  | 12 (12%) | 8 (8%)   | 1           | 11 |
| 42  | RW    | 111/113 (98%) | 99 (89%)  | 8 (7%)   | 4 (4%)   | 3           | 29 |
| 42  | YW    | 111/113 (98%) | 100 (90%) | 9 (8%)   | 2 (2%)   | 8           | 43 |
| 43  | RX    | 90/96 (94%)   | 77 (86%)  | 11 (12%) | 2 (2%)   | 6           | 39 |
| 43  | YX    | 90/96 (94%)   | 82 (91%)  | 6 (7%)   | 2 (2%)   | 6           | 39 |
| 44  | RY    | 100/110 (91%) | 71 (71%)  | 13 (13%) | 16 (16%) | 0           | 3  |
| 44  | YY    | 100/110 (91%) | 70 (70%)  | 18 (18%) | 12 (12%) | 0           | 5  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 45  | RZ    | 181/206 (88%)     | 126 (70%)  | 34 (19%)   | 21 (12%) | 0           | 6   |
| 45  | YZ    | 181/206 (88%)     | 125 (69%)  | 38 (21%)   | 18 (10%) | 0           | 8   |
| 46  | R0    | 80/85 (94%)       | 65 (81%)   | 14 (18%)   | 1 (1%)   | 12          | 50  |
| 46  | Y0    | 80/85 (94%)       | 73 (91%)   | 7 (9%)     | 0        | 100         | 100 |
| 47  | R1    | 95/98 (97%)       | 76 (80%)   | 10 (10%)   | 9 (10%)  | 0           | 8   |
| 47  | Y1    | 95/98 (97%)       | 72 (76%)   | 17 (18%)   | 6 (6%)   | 1           | 17  |
| 48  | R2    | 67/72 (93%)       | 53 (79%)   | 9 (13%)    | 5 (8%)   | 1           | 12  |
| 48  | Y2    | 67/72 (93%)       | 55 (82%)   | 6 (9%)     | 6 (9%)   | 1           | 9   |
| 49  | R3    | 57/60 (95%)       | 52 (91%)   | 3 (5%)     | 2 (4%)   | 3           | 30  |
| 49  | Y3    | 57/60 (95%)       | 52 (91%)   | 4 (7%)     | 1 (2%)   | 8           | 43  |
| 50  | R4    | 69/71 (97%)       | 35 (51%)   | 18 (26%)   | 16 (23%) | 0           | 0   |
| 50  | Y4    | 69/71 (97%)       | 35 (51%)   | 15 (22%)   | 19 (28%) | 0           | 0   |
| 51  | R5    | 57/60 (95%)       | 47 (82%)   | 7 (12%)    | 3 (5%)   | 2           | 19  |
| 51  | Y5    | 55/60 (92%)       | 45 (82%)   | 9 (16%)    | 1 (2%)   | 8           | 43  |
| 52  | R6    | 47/54 (87%)       | 23 (49%)   | 13 (28%)   | 11 (23%) | 0           | 0   |
| 52  | Y6    | 47/54 (87%)       | 22 (47%)   | 17 (36%)   | 8 (17%)  | 0           | 2   |
| 53  | R7    | 47/49 (96%)       | 45 (96%)   | 1 (2%)     | 1 (2%)   | 7           | 40  |
| 53  | Y7    | 47/49 (96%)       | 43 (92%)   | 3 (6%)     | 1 (2%)   | 7           | 40  |
| 54  | R8    | 62/65 (95%)       | 51 (82%)   | 6 (10%)    | 5 (8%)   | 1           | 11  |
| 54  | Y8    | 62/65 (95%)       | 48 (77%)   | 10 (16%)   | 4 (6%)   | 1           | 16  |
| 55  | R9    | 35/37 (95%)       | 35 (100%)  | 0          | 0        | 100         | 100 |
| 55  | Y9    | 35/37 (95%)       | 31 (89%)   | 4 (11%)    | 0        | 100         | 100 |
| 56  | Z7    | 7/12 (58%)        | 5 (71%)    | 2 (29%)    | 0        | 100         | 100 |
| 56  | Z8    | 7/12 (58%)        | 3 (43%)    | 3 (43%)    | 1 (14%)  | 0           | 4   |
| All | All   | 11482/12152 (94%) | 9247 (80%) | 1516 (13%) | 719 (6%) | 1           | 17  |

All (719) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 236 | TYR  |
| 3   | QC    | 12  | LEU  |
| 3   | QC    | 190 | ARG  |
| 4   | QD    | 28  | SER  |
| 6   | QF    | 16  | GLN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 6          | QF           | 17         | SER         |
| 6          | QF           | 18         | GLN         |
| 13         | QM           | 67         | GLU         |
| 13         | QM           | 106        | ASN         |
| 13         | QM           | 118        | ALA         |
| 14         | QN           | 16         | PHE         |
| 19         | QS           | 12         | ASP         |
| 19         | QS           | 45         | VAL         |
| 20         | QT           | 49         | ALA         |
| 27         | RD           | 26         | LYS         |
| 27         | RD           | 122        | ASP         |
| 27         | RD           | 242        | ARG         |
| 28         | RE           | 53         | PRO         |
| 28         | RE           | 63         | LEU         |
| 28         | RE           | 68         | ALA         |
| 28         | RE           | 71         | GLY         |
| 28         | RE           | 93         | VAL         |
| 31         | RH           | 12         | PRO         |
| 31         | RH           | 86         | GLU         |
| 31         | RH           | 126        | PRO         |
| 31         | RH           | 154        | PRO         |
| 31         | RH           | 168        | PRO         |
| 31         | RH           | 169        | VAL         |
| 32         | RI           | 115        | ALA         |
| 32         | RI           | 133        | HIS         |
| 33         | RN           | 9          | VAL         |
| 33         | RN           | 22         | THR         |
| 33         | RN           | 96         | GLU         |
| 33         | RN           | 131        | GLN         |
| 34         | RO           | 5          | GLN         |
| 35         | RP           | 6          | LEU         |
| 35         | RP           | 10         | PRO         |
| 35         | RP           | 11         | GLY         |
| 35         | RP           | 15         | ARG         |
| 35         | RP           | 65         | ARG         |
| 35         | RP           | 95         | VAL         |
| 35         | RP           | 141        | ALA         |
| 35         | RP           | 148        | LEU         |
| 36         | RQ           | 22         | LYS         |
| 36         | RQ           | 66         | ILE         |
| 36         | RQ           | 78         | PRO         |
| 36         | RQ           | 90         | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | RQ    | 139 | GLU  |
| 37  | RR    | 3   | HIS  |
| 37  | RR    | 4   | LEU  |
| 38  | RS    | 57  | LYS  |
| 38  | RS    | 88  | ASP  |
| 38  | RS    | 89  | ARG  |
| 39  | RT    | 2   | ASN  |
| 39  | RT    | 3   | ARG  |
| 39  | RT    | 106 | SER  |
| 39  | RT    | 112 | ARG  |
| 39  | RT    | 124 | ASP  |
| 40  | RU    | 91  | ASP  |
| 41  | RV    | 48  | GLY  |
| 41  | RV    | 50  | PRO  |
| 41  | RV    | 100 | ARG  |
| 42  | RW    | 111 | HIS  |
| 44  | RY    | 3   | VAL  |
| 44  | RY    | 50  | ARG  |
| 44  | RY    | 57  | GLN  |
| 44  | RY    | 77  | PRO  |
| 44  | RY    | 78  | ALA  |
| 45  | RZ    | 13  | GLU  |
| 45  | RZ    | 111 | VAL  |
| 48  | R2    | 47  | ASN  |
| 48  | R2    | 48  | HIS  |
| 48  | R2    | 70  | GLN  |
| 48  | R2    | 71  | ASN  |
| 50  | R4    | 16  | CYS  |
| 50  | R4    | 18  | CYS  |
| 50  | R4    | 40  | HIS  |
| 50  | R4    | 43  | TYR  |
| 50  | R4    | 49  | PHE  |
| 50  | R4    | 50  | VAL  |
| 50  | R4    | 53  | GLU  |
| 51  | R5    | 4   | HIS  |
| 51  | R5    | 53  | ALA  |
| 52  | R6    | 15  | GLU  |
| 54  | R8    | 34  | TRP  |
| 54  | R8    | 52  | LYS  |
| 54  | R8    | 62  | LEU  |
| 2   | XB    | 230 | VAL  |
| 2   | XB    | 236 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | XC    | 12  | LEU  |
| 3   | XC    | 79  | ARG  |
| 4   | XD    | 154 | ASN  |
| 11  | XK    | 91  | ARG  |
| 12  | XL    | 47  | LYS  |
| 12  | XL    | 49  | ASN  |
| 12  | XL    | 51  | ALA  |
| 12  | XL    | 64  | TYR  |
| 13  | XM    | 67  | GLU  |
| 13  | XM    | 106 | ASN  |
| 13  | XM    | 118 | ALA  |
| 14  | XN    | 14  | PRO  |
| 14  | XN    | 16  | PHE  |
| 14  | XN    | 52  | GLN  |
| 19  | XS    | 3   | ARG  |
| 19  | XS    | 12  | ASP  |
| 20  | XT    | 48  | LYS  |
| 20  | XT    | 96  | GLY  |
| 27  | YD    | 26  | LYS  |
| 27  | YD    | 28  | GLU  |
| 27  | YD    | 122 | ASP  |
| 27  | YD    | 123 | ALA  |
| 28  | YE    | 2   | LYS  |
| 28  | YE    | 19  | ARG  |
| 28  | YE    | 53  | PRO  |
| 28  | YE    | 63  | LEU  |
| 28  | YE    | 71  | GLY  |
| 29  | YF    | 73  | ALA  |
| 29  | YF    | 134 | GLY  |
| 30  | YG    | 96  | ARG  |
| 31  | YH    | 3   | ARG  |
| 31  | YH    | 12  | PRO  |
| 31  | YH    | 86  | GLU  |
| 31  | YH    | 126 | PRO  |
| 31  | YH    | 127 | GLU  |
| 31  | YH    | 128 | PRO  |
| 31  | YH    | 153 | LYS  |
| 31  | YH    | 155 | SER  |
| 31  | YH    | 168 | PRO  |
| 31  | YH    | 169 | VAL  |
| 32  | YI    | 133 | HIS  |
| 32  | YI    | 145 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | YN    | 9   | VAL  |
| 33  | YN    | 22  | THR  |
| 33  | YN    | 36  | GLY  |
| 35  | YP    | 6   | LEU  |
| 35  | YP    | 10  | PRO  |
| 35  | YP    | 14  | LYS  |
| 35  | YP    | 15  | ARG  |
| 35  | YP    | 25  | SER  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 95  | VAL  |
| 35  | YP    | 106 | LEU  |
| 35  | YP    | 148 | LEU  |
| 36  | YQ    | 18  | LYS  |
| 36  | YQ    | 22  | LYS  |
| 36  | YQ    | 25  | ASP  |
| 36  | YQ    | 79  | LEU  |
| 36  | YQ    | 86  | GLY  |
| 36  | YQ    | 90  | VAL  |
| 36  | YQ    | 134 | ARG  |
| 37  | YR    | 3   | HIS  |
| 38  | YS    | 82  | ILE  |
| 38  | YS    | 88  | ASP  |
| 38  | YS    | 107 | GLU  |
| 39  | YT    | 2   | ASN  |
| 39  | YT    | 123 | GLN  |
| 39  | YT    | 124 | ASP  |
| 40  | YU    | 90  | VAL  |
| 40  | YU    | 91  | ASP  |
| 40  | YU    | 93  | LYS  |
| 41  | YV    | 45  | THR  |
| 43  | YX    | 68  | ARG  |
| 44  | YY    | 50  | ARG  |
| 44  | YY    | 57  | GLN  |
| 44  | YY    | 77  | PRO  |
| 44  | YY    | 78  | ALA  |
| 45  | YZ    | 6   | LYS  |
| 45  | YZ    | 53  | ILE  |
| 45  | YZ    | 146 | ILE  |
| 45  | YZ    | 152 | ALA  |
| 45  | YZ    | 159 | PRO  |
| 47  | Y1    | 30  | VAL  |
| 47  | Y1    | 84  | GLY  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 47         | Y1           | 91         | LYS         |
| 47         | Y1           | 95         | LEU         |
| 48         | Y2           | 16         | LEU         |
| 48         | Y2           | 43         | GLN         |
| 48         | Y2           | 47         | ASN         |
| 48         | Y2           | 48         | HIS         |
| 50         | Y4           | 24         | THR         |
| 50         | Y4           | 40         | HIS         |
| 50         | Y4           | 49         | PHE         |
| 51         | Y5           | 4          | HIS         |
| 52         | Y6           | 15         | GLU         |
| 53         | Y7           | 48         | LYS         |
| 54         | Y8           | 52         | LYS         |
| 54         | Y8           | 62         | LEU         |
| 2          | QB           | 15         | VAL         |
| 2          | QB           | 96         | ARG         |
| 2          | QB           | 229        | VAL         |
| 2          | QB           | 230        | VAL         |
| 2          | QB           | 237        | ALA         |
| 3          | QC           | 79         | ARG         |
| 4          | QD           | 51         | PRO         |
| 4          | QD           | 154        | ASN         |
| 5          | QE           | 115        | VAL         |
| 8          | QH           | 129        | VAL         |
| 9          | QI           | 41         | VAL         |
| 9          | QI           | 117        | HIS         |
| 11         | QK           | 101        | SER         |
| 12         | QL           | 47         | LYS         |
| 12         | QL           | 91         | LYS         |
| 13         | QM           | 12         | ASN         |
| 14         | QN           | 12         | ARG         |
| 17         | QQ           | 74         | LEU         |
| 17         | QQ           | 81         | ARG         |
| 19         | QS           | 3          | ARG         |
| 19         | QS           | 11         | VAL         |
| 19         | QS           | 26         | GLY         |
| 19         | QS           | 31         | ILE         |
| 19         | QS           | 41         | VAL         |
| 27         | RD           | 32         | SER         |
| 28         | RE           | 50         | GLY         |
| 28         | RE           | 60         | ASN         |
| 28         | RE           | 66         | HIS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | RE    | 72  | VAL  |
| 28  | RE    | 90  | THR  |
| 28  | RE    | 92  | THR  |
| 28  | RE    | 187 | ALA  |
| 29  | RF    | 17  | ARG  |
| 29  | RF    | 67  | GLN  |
| 29  | RF    | 73  | ALA  |
| 29  | RF    | 89  | VAL  |
| 29  | RF    | 134 | GLY  |
| 29  | RF    | 198 | ALA  |
| 30  | RG    | 4   | ASP  |
| 30  | RG    | 5   | VAL  |
| 30  | RG    | 14  | GLU  |
| 30  | RG    | 96  | ARG  |
| 30  | RG    | 137 | GLU  |
| 30  | RG    | 146 | TYR  |
| 31  | RH    | 137 | ASP  |
| 31  | RH    | 153 | LYS  |
| 31  | RH    | 155 | SER  |
| 32  | RI    | 10  | GLU  |
| 32  | RI    | 11  | ASN  |
| 32  | RI    | 102 | SER  |
| 32  | RI    | 117 | GLU  |
| 32  | RI    | 145 | VAL  |
| 35  | RP    | 90  | ARG  |
| 35  | RP    | 103 | ALA  |
| 35  | RP    | 106 | LEU  |
| 36  | RQ    | 6   | ARG  |
| 36  | RQ    | 25  | ASP  |
| 36  | RQ    | 27  | VAL  |
| 36  | RQ    | 133 | ARG  |
| 37  | RR    | 107 | ASP  |
| 38  | RS    | 4   | LEU  |
| 38  | RS    | 107 | GLU  |
| 39  | RT    | 37  | GLY  |
| 40  | RU    | 90  | VAL  |
| 41  | RV    | 49  | THR  |
| 41  | RV    | 79  | VAL  |
| 43  | RX    | 41  | ASN  |
| 44  | RY    | 45  | VAL  |
| 44  | RY    | 48  | ALA  |
| 44  | RY    | 63  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | RZ    | 6   | LYS  |
| 45  | RZ    | 53  | ILE  |
| 45  | RZ    | 92  | SER  |
| 45  | RZ    | 153 | SER  |
| 45  | RZ    | 177 | PRO  |
| 45  | RZ    | 179 | ASP  |
| 47  | R1    | 30  | VAL  |
| 47  | R1    | 80  | LEU  |
| 47  | R1    | 84  | GLY  |
| 47  | R1    | 91  | LYS  |
| 47  | R1    | 95  | LEU  |
| 48  | R2    | 43  | GLN  |
| 49  | R3    | 26  | LEU  |
| 50  | R4    | 24  | THR  |
| 50  | R4    | 30  | GLU  |
| 50  | R4    | 51  | ASP  |
| 50  | R4    | 66  | SER  |
| 51  | R5    | 59  | GLU  |
| 52  | R6    | 7   | ILE  |
| 52  | R6    | 45  | LYS  |
| 2   | XB    | 15  | VAL  |
| 4   | XD    | 30  | LYS  |
| 4   | XD    | 166 | LYS  |
| 5   | XE    | 115 | VAL  |
| 7   | XG    | 55  | GLY  |
| 8   | XH    | 50  | ARG  |
| 9   | XI    | 41  | VAL  |
| 9   | XI    | 127 | LYS  |
| 10  | XJ    | 30  | SER  |
| 10  | XJ    | 86  | MET  |
| 12  | XL    | 63  | GLY  |
| 12  | XL    | 91  | LYS  |
| 12  | XL    | 115 | LYS  |
| 13  | XM    | 6   | GLY  |
| 13  | XM    | 21  | TYR  |
| 19  | XS    | 41  | VAL  |
| 19  | XS    | 45  | VAL  |
| 20  | XT    | 99  | LEU  |
| 27  | YD    | 238 | GLY  |
| 27  | YD    | 242 | ARG  |
| 28  | YE    | 7   | VAL  |
| 28  | YE    | 204 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | YF    | 128 | ALA  |
| 29  | YF    | 132 | VAL  |
| 29  | YF    | 181 | LEU  |
| 30  | YG    | 4   | ASP  |
| 30  | YG    | 36  | LYS  |
| 31  | YH    | 13  | LYS  |
| 31  | YH    | 27  | LYS  |
| 31  | YH    | 50  | VAL  |
| 31  | YH    | 85  | LYS  |
| 33  | YN    | 23  | LEU  |
| 33  | YN    | 96  | GLU  |
| 34  | YO    | 5   | GLN  |
| 35  | YP    | 65  | ARG  |
| 35  | YP    | 66  | GLY  |
| 35  | YP    | 93  | GLY  |
| 35  | YP    | 141 | ALA  |
| 36  | YQ    | 6   | ARG  |
| 36  | YQ    | 60  | ARG  |
| 36  | YQ    | 137 | TYR  |
| 37  | YR    | 4   | LEU  |
| 37  | YR    | 45  | ARG  |
| 37  | YR    | 107 | ASP  |
| 38  | YS    | 12  | PHE  |
| 38  | YS    | 56  | LEU  |
| 38  | YS    | 109 | GLY  |
| 39  | YT    | 13  | ARG  |
| 39  | YT    | 39  | ARG  |
| 39  | YT    | 106 | SER  |
| 41  | YV    | 31  | ALA  |
| 41  | YV    | 48  | GLY  |
| 41  | YV    | 79  | VAL  |
| 42  | YW    | 111 | HIS  |
| 44  | YY    | 58  | GLY  |
| 44  | YY    | 102 | CYS  |
| 45  | YZ    | 13  | GLU  |
| 45  | YZ    | 81  | ARG  |
| 48  | Y2    | 70  | GLN  |
| 48  | Y2    | 71  | ASN  |
| 50  | Y4    | 5   | ILE  |
| 50  | Y4    | 18  | CYS  |
| 50  | Y4    | 22  | ILE  |
| 50  | Y4    | 37  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Y4    | 43  | TYR  |
| 50  | Y4    | 50  | VAL  |
| 52  | Y6    | 7   | ILE  |
| 52  | Y6    | 16  | CYS  |
| 52  | Y6    | 33  | LYS  |
| 2   | QB    | 26  | PRO  |
| 2   | QB    | 87  | ARG  |
| 2   | QB    | 204 | ASN  |
| 2   | QB    | 207 | ALA  |
| 3   | QC    | 4   | LYS  |
| 3   | QC    | 51  | GLY  |
| 4   | QD    | 155 | LEU  |
| 5   | QE    | 77  | PRO  |
| 10  | QJ    | 30  | SER  |
| 11  | QK    | 103 | LEU  |
| 11  | QK    | 125 | PHE  |
| 12  | QL    | 28  | LYS  |
| 13  | QM    | 120 | LYS  |
| 14  | QN    | 14  | PRO  |
| 15  | QO    | 23  | GLY  |
| 19  | QS    | 9   | VAL  |
| 19  | QS    | 14  | HIS  |
| 19  | QS    | 28  | LYS  |
| 20  | QT    | 96  | GLY  |
| 27  | RD    | 46  | GLN  |
| 27  | RD    | 239 | ARG  |
| 28  | RE    | 79  | ARG  |
| 28  | RE    | 204 | ALA  |
| 29  | RF    | 133 | ASN  |
| 30  | RG    | 32  | PRO  |
| 30  | RG    | 116 | ASP  |
| 31  | RH    | 5   | GLY  |
| 31  | RH    | 8   | PRO  |
| 31  | RH    | 27  | LYS  |
| 31  | RH    | 55  | PRO  |
| 31  | RH    | 87  | LEU  |
| 31  | RH    | 138 | LYS  |
| 32  | RI    | 15  | VAL  |
| 32  | RI    | 118 | LYS  |
| 33  | RN    | 8   | GLN  |
| 33  | RN    | 23  | LEU  |
| 33  | RN    | 95  | PRO  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 33         | RN           | 130        | HIS         |
| 34         | RO           | 97         | ARG         |
| 35         | RP           | 29         | LYS         |
| 35         | RP           | 67         | MET         |
| 36         | RQ           | 11         | LYS         |
| 36         | RQ           | 19         | GLY         |
| 36         | RQ           | 137        | TYR         |
| 37         | RR           | 74         | LYS         |
| 38         | RS           | 12         | PHE         |
| 38         | RS           | 61         | ASN         |
| 39         | RT           | 12         | SER         |
| 39         | RT           | 97         | ALA         |
| 40         | RU           | 117        | GLN         |
| 44         | RY           | 58         | GLY         |
| 45         | RZ           | 7          | ALA         |
| 45         | RZ           | 66         | SER         |
| 45         | RZ           | 116        | VAL         |
| 45         | RZ           | 119        | GLU         |
| 45         | RZ           | 152        | ALA         |
| 47         | R1           | 76         | ARG         |
| 49         | R3           | 27         | GLY         |
| 52         | R6           | 33         | LYS         |
| 52         | R6           | 35         | GLU         |
| 52         | R6           | 49         | HIS         |
| 54         | R8           | 31         | HIS         |
| 54         | R8           | 51         | ALA         |
| 2          | XB           | 13         | ALA         |
| 2          | XB           | 22         | LYS         |
| 2          | XB           | 24         | TRP         |
| 2          | XB           | 135        | GLN         |
| 2          | XB           | 207        | ALA         |
| 4          | XD           | 73         | ARG         |
| 4          | XD           | 155        | LEU         |
| 7          | XG           | 7          | ALA         |
| 8          | XH           | 2          | LEU         |
| 9          | XI           | 56         | LEU         |
| 9          | XI           | 95         | LYS         |
| 10         | XJ           | 59         | SER         |
| 11         | XK           | 103        | LEU         |
| 13         | XM           | 4          | ILE         |
| 13         | XM           | 12         | ASN         |
| 13         | XM           | 42         | ALA         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 19         | XS           | 27         | GLU         |
| 19         | XS           | 28         | LYS         |
| 27         | YD           | 32         | SER         |
| 28         | YE           | 50         | GLY         |
| 28         | YE           | 79         | ARG         |
| 28         | YE           | 90         | THR         |
| 28         | YE           | 92         | THR         |
| 28         | YE           | 117        | MET         |
| 28         | YE           | 184        | VAL         |
| 29         | YF           | 198        | ALA         |
| 31         | YH           | 87         | LEU         |
| 31         | YH           | 137        | ASP         |
| 31         | YH           | 138        | LYS         |
| 31         | YH           | 151        | ILE         |
| 32         | YI           | 11         | ASN         |
| 32         | YI           | 12         | LEU         |
| 32         | YI           | 72         | LEU         |
| 32         | YI           | 113        | ARG         |
| 32         | YI           | 122        | GLU         |
| 33         | YN           | 7          | LYS         |
| 33         | YN           | 131        | GLN         |
| 35         | YP           | 16         | ARG         |
| 35         | YP           | 29         | LYS         |
| 36         | YQ           | 19         | GLY         |
| 36         | YQ           | 105        | GLU         |
| 36         | YQ           | 133        | ARG         |
| 37         | YR           | 86         | ARG         |
| 38         | YS           | 4          | LEU         |
| 38         | YS           | 11         | LYS         |
| 38         | YS           | 60         | GLY         |
| 39         | YT           | 97         | ALA         |
| 41         | YV           | 49         | THR         |
| 41         | YV           | 53         | GLU         |
| 41         | YV           | 100        | ARG         |
| 44         | YY           | 42         | VAL         |
| 44         | YY           | 63         | LYS         |
| 45         | YZ           | 59         | LEU         |
| 45         | YZ           | 92         | SER         |
| 45         | YZ           | 160        | GLY         |
| 45         | YZ           | 166        | SER         |
| 49         | Y3           | 3          | ARG         |
| 50         | Y4           | 23         | GLU         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Y4    | 30  | GLU  |
| 50  | Y4    | 34  | GLU  |
| 50  | Y4    | 66  | SER  |
| 52  | Y6    | 19  | ARG  |
| 52  | Y6    | 49  | HIS  |
| 54  | Y8    | 30  | ARG  |
| 54  | Y8    | 34  | TRP  |
| 56  | Z8    | 2   | GLY  |
| 2   | QB    | 22  | LYS  |
| 2   | QB    | 126 | GLU  |
| 2   | QB    | 209 | ARG  |
| 4   | QD    | 171 | GLY  |
| 9   | QI    | 56  | LEU  |
| 12  | QL    | 27  | LEU  |
| 12  | QL    | 48  | PRO  |
| 13  | QM    | 6   | GLY  |
| 13  | QM    | 13  | LYS  |
| 18  | QR    | 20  | ALA  |
| 18  | QR    | 54  | ARG  |
| 20  | QT    | 71  | THR  |
| 21  | QU    | 9   | ARG  |
| 27  | RD    | 3   | VAL  |
| 27  | RD    | 123 | ALA  |
| 27  | RD    | 237 | GLU  |
| 28  | RE    | 78  | LEU  |
| 29  | RF    | 66  | PRO  |
| 29  | RF    | 197 | ASP  |
| 30  | RG    | 36  | LYS  |
| 30  | RG    | 86  | MET  |
| 31  | RH    | 92  | ILE  |
| 32  | RI    | 122 | GLU  |
| 35  | RP    | 21  | ARG  |
| 36  | RQ    | 21  | THR  |
| 36  | RQ    | 28  | ALA  |
| 36  | RQ    | 86  | GLY  |
| 36  | RQ    | 104 | PHE  |
| 36  | RQ    | 105 | GLU  |
| 37  | RR    | 71  | GLN  |
| 38  | RS    | 109 | GLY  |
| 39  | RT    | 38  | ASN  |
| 39  | RT    | 39  | ARG  |
| 40  | RU    | 98  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | RW    | 18  | ARG  |
| 42  | RW    | 63  | ASP  |
| 42  | RW    | 68  | ARG  |
| 43  | RX    | 67  | GLY  |
| 44  | RY    | 4   | LYS  |
| 44  | RY    | 53  | PRO  |
| 44  | RY    | 99  | CYS  |
| 45  | RZ    | 165 | VAL  |
| 52  | R6    | 16  | CYS  |
| 53  | R7    | 48  | LYS  |
| 2   | XB    | 19  | HIS  |
| 2   | XB    | 101 | MET  |
| 2   | XB    | 155 | LEU  |
| 5   | XE    | 70  | PRO  |
| 8   | XH    | 129 | VAL  |
| 12  | XL    | 19  | ARG  |
| 12  | XL    | 28  | LYS  |
| 14  | XN    | 15  | LYS  |
| 14  | XN    | 32  | SER  |
| 15  | XO    | 88  | ARG  |
| 18  | XR    | 20  | ALA  |
| 19  | XS    | 9   | VAL  |
| 20  | XT    | 84  | LEU  |
| 20  | XT    | 98  | PRO  |
| 21  | XU    | 9   | ARG  |
| 30  | YG    | 14  | GLU  |
| 30  | YG    | 82  | LEU  |
| 30  | YG    | 86  | MET  |
| 30  | YG    | 116 | ASP  |
| 31  | YH    | 8   | PRO  |
| 31  | YH    | 83  | TYR  |
| 32  | YI    | 10  | GLU  |
| 32  | YI    | 87  | LYS  |
| 32  | YI    | 114 | LEU  |
| 33  | YN    | 11  | PRO  |
| 33  | YN    | 28  | THR  |
| 33  | YN    | 47  | ALA  |
| 36  | YQ    | 104 | PHE  |
| 36  | YQ    | 140 | ALA  |
| 38  | YS    | 89  | ARG  |
| 38  | YS    | 96  | GLY  |
| 39  | YT    | 17  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | YX    | 40  | LYS  |
| 44  | YY    | 51  | VAL  |
| 44  | YY    | 53  | PRO  |
| 50  | Y4    | 9   | LEU  |
| 50  | Y4    | 16  | CYS  |
| 50  | Y4    | 25  | TYR  |
| 50  | Y4    | 54  | GLY  |
| 52  | Y6    | 35  | GLU  |
| 2   | QB    | 234 | PRO  |
| 4   | QD    | 30  | LYS  |
| 4   | QD    | 42  | GLN  |
| 5   | QE    | 70  | PRO  |
| 5   | QE    | 96  | PRO  |
| 7   | QG    | 7   | ALA  |
| 9   | QI    | 121 | ARG  |
| 12  | QL    | 19  | ARG  |
| 12  | QL    | 121 | GLY  |
| 13  | QM    | 4   | ILE  |
| 18  | QR    | 26  | LEU  |
| 20  | QT    | 73  | HIS  |
| 20  | QT    | 97  | ALA  |
| 27  | RD    | 238 | GLY  |
| 28  | RE    | 21  | VAL  |
| 28  | RE    | 54  | GLN  |
| 29  | RF    | 8   | GLN  |
| 30  | RG    | 82  | LEU  |
| 31  | RH    | 21  | PRO  |
| 31  | RH    | 83  | TYR  |
| 32  | RI    | 12  | LEU  |
| 32  | RI    | 30  | LEU  |
| 33  | RN    | 18  | ALA  |
| 33  | RN    | 57  | ALA  |
| 33  | RN    | 135 | PRO  |
| 38  | RS    | 97  | ARG  |
| 38  | RS    | 110 | LEU  |
| 44  | RY    | 5   | MET  |
| 44  | RY    | 39  | VAL  |
| 44  | RY    | 41  | GLY  |
| 44  | RY    | 62  | GLU  |
| 45  | RZ    | 12  | GLY  |
| 45  | RZ    | 51  | ALA  |
| 45  | RZ    | 61  | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 45         | RZ           | 158        | PRO         |
| 45         | RZ           | 181        | GLU         |
| 46         | R0           | 18         | ALA         |
| 47         | R1           | 74         | VAL         |
| 47         | R1           | 82         | LEU         |
| 50         | R4           | 5          | ILE         |
| 50         | R4           | 23         | GLU         |
| 50         | R4           | 28         | LYS         |
| 50         | R4           | 68         | ARG         |
| 52         | R6           | 9          | LEU         |
| 52         | R6           | 19         | ARG         |
| 2          | XB           | 121        | LEU         |
| 3          | XC           | 181        | ASN         |
| 10         | XJ           | 27         | ALA         |
| 12         | XL           | 27         | LEU         |
| 12         | XL           | 65         | GLU         |
| 13         | XM           | 101        | GLN         |
| 15         | XO           | 23         | GLY         |
| 20         | XT           | 97         | ALA         |
| 27         | YD           | 3          | VAL         |
| 27         | YD           | 46         | GLN         |
| 28         | YE           | 68         | ALA         |
| 28         | YE           | 82         | ARG         |
| 28         | YE           | 86         | PRO         |
| 30         | YG           | 5          | VAL         |
| 30         | YG           | 53         | LEU         |
| 30         | YG           | 117        | PHE         |
| 32         | YI           | 18         | VAL         |
| 32         | YI           | 71         | ILE         |
| 32         | YI           | 117        | GLU         |
| 32         | YI           | 118        | LYS         |
| 33         | YN           | 95         | PRO         |
| 33         | YN           | 134        | ARG         |
| 33         | YN           | 135        | PRO         |
| 35         | YP           | 11         | GLY         |
| 35         | YP           | 24         | GLY         |
| 36         | YQ           | 11         | LYS         |
| 36         | YQ           | 27         | VAL         |
| 38         | YS           | 94         | TYR         |
| 38         | YS           | 110        | LEU         |
| 39         | YT           | 86         | ILE         |
| 40         | YU           | 117        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 41         | YV           | 50         | PRO         |
| 44         | YY           | 3          | VAL         |
| 44         | YY           | 39         | VAL         |
| 45         | YZ           | 51         | ALA         |
| 45         | YZ           | 61         | LEU         |
| 45         | YZ           | 62         | PRO         |
| 45         | YZ           | 168        | GLU         |
| 45         | YZ           | 181        | GLU         |
| 47         | Y1           | 74         | VAL         |
| 50         | Y4           | 14         | ILE         |
| 52         | Y6           | 21         | TYR         |
| 2          | QB           | 155        | LEU         |
| 10         | QJ           | 82         | ILE         |
| 13         | QM           | 10         | PRO         |
| 14         | QN           | 15         | LYS         |
| 20         | QT           | 98         | PRO         |
| 27         | RD           | 125        | ILE         |
| 28         | RE           | 82         | ARG         |
| 29         | RF           | 130        | ALA         |
| 30         | RG           | 52         | ILE         |
| 30         | RG           | 88         | ILE         |
| 30         | RG           | 117        | PHE         |
| 38         | RS           | 82         | ILE         |
| 39         | RT           | 40         | THR         |
| 45         | RZ           | 62         | PRO         |
| 45         | RZ           | 166        | SER         |
| 47         | R1           | 55         | GLY         |
| 50         | R4           | 11         | PRO         |
| 52         | R6           | 21         | TYR         |
| 52         | R6           | 34         | LEU         |
| 2          | XB           | 26         | PRO         |
| 2          | XB           | 126        | GLU         |
| 2          | XB           | 237        | ALA         |
| 10         | XJ           | 91         | PRO         |
| 13         | XM           | 7          | VAL         |
| 14         | XN           | 60         | SER         |
| 19         | XS           | 7          | LYS         |
| 28         | YE           | 72         | VAL         |
| 29         | YF           | 58         | ALA         |
| 33         | YN           | 127        | ASP         |
| 34         | YO           | 97         | ARG         |
| 35         | YP           | 7          | ARG         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | YQ    | 62  | GLY  |
| 47  | Y1    | 55  | GLY  |
| 50  | Y4    | 60  | GLN  |
| 2   | QB    | 5   | ILE  |
| 16  | QP    | 46  | PRO  |
| 28  | RE    | 86  | PRO  |
| 31  | RH    | 166 | GLY  |
| 36  | RQ    | 81  | VAL  |
| 5   | XE    | 74  | GLY  |
| 12  | XL    | 18  | VAL  |
| 32  | YI    | 15  | VAL  |
| 36  | YQ    | 81  | VAL  |
| 3   | QC    | 81  | GLY  |
| 5   | QE    | 74  | GLY  |
| 19  | QS    | 46  | GLY  |
| 27  | RD    | 35  | LYS  |
| 32  | RI    | 13  | GLY  |
| 19  | XS    | 26  | GLY  |
| 19  | XS    | 46  | GLY  |
| 29  | YF    | 66  | PRO  |
| 32  | YI    | 16  | GLY  |
| 39  | YT    | 37  | GLY  |
| 42  | YW    | 14  | PRO  |
| 45  | YZ    | 101 | PRO  |
| 7   | QG    | 50  | ILE  |
| 9   | QI    | 89  | ASN  |
| 10  | QJ    | 37  | PRO  |
| 33  | RN    | 134 | ARG  |
| 39  | RT    | 86  | ILE  |
| 8   | XH    | 51  | VAL  |
| 16  | XP    | 46  | PRO  |
| 19  | XS    | 31  | ILE  |
| 32  | YI    | 13  | GLY  |
| 29  | RF    | 132 | VAL  |
| 41  | RV    | 54  | GLY  |
| 30  | YG    | 52  | ILE  |
| 30  | YG    | 88  | ILE  |
| 31  | YH    | 7   | LEU  |
| 37  | YR    | 117 | VAL  |
| 2   | QB    | 227 | GLY  |
| 45  | YZ    | 94  | GLU  |
| 28  | RE    | 22  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | QB    | 205/220 (93%)  | 171 (83%) | 34 (17%) | 2           | 15 |
| 2   | XB    | 205/220 (93%)  | 180 (88%) | 25 (12%) | 5           | 26 |
| 3   | QC    | 159/188 (85%)  | 145 (91%) | 14 (9%)  | 10          | 40 |
| 3   | XC    | 159/188 (85%)  | 146 (92%) | 13 (8%)  | 11          | 42 |
| 4   | QD    | 180/181 (99%)  | 157 (87%) | 23 (13%) | 4           | 24 |
| 4   | XD    | 180/181 (99%)  | 152 (84%) | 28 (16%) | 2           | 18 |
| 5   | QE    | 116/123 (94%)  | 104 (90%) | 12 (10%) | 7           | 34 |
| 5   | XE    | 116/123 (94%)  | 104 (90%) | 12 (10%) | 7           | 34 |
| 6   | QF    | 90/90 (100%)   | 78 (87%)  | 12 (13%) | 4           | 23 |
| 6   | XF    | 90/90 (100%)   | 81 (90%)  | 9 (10%)  | 7           | 35 |
| 7   | QG    | 126/127 (99%)  | 114 (90%) | 12 (10%) | 8           | 37 |
| 7   | XG    | 126/127 (99%)  | 114 (90%) | 12 (10%) | 8           | 37 |
| 8   | QH    | 119/119 (100%) | 109 (92%) | 10 (8%)  | 11          | 42 |
| 8   | XH    | 119/119 (100%) | 106 (89%) | 13 (11%) | 6           | 32 |
| 9   | QI    | 98/99 (99%)    | 81 (83%)  | 17 (17%) | 2           | 12 |
| 9   | XI    | 98/99 (99%)    | 80 (82%)  | 18 (18%) | 1           | 10 |
| 10  | QJ    | 89/92 (97%)    | 77 (86%)  | 12 (14%) | 4           | 23 |
| 10  | XJ    | 89/92 (97%)    | 74 (83%)  | 15 (17%) | 2           | 14 |
| 11  | QK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 7           | 35 |
| 11  | XK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 7           | 35 |
| 12  | QL    | 104/109 (95%)  | 87 (84%)  | 17 (16%) | 2           | 15 |
| 12  | XL    | 104/109 (95%)  | 92 (88%)  | 12 (12%) | 5           | 29 |
| 13  | QM    | 97/101 (96%)   | 73 (75%)  | 24 (25%) | 0           | 4  |
| 13  | XM    | 97/101 (96%)   | 78 (80%)  | 19 (20%) | 1           | 8  |
| 14  | QN    | 49/50 (98%)    | 40 (82%)  | 9 (18%)  | 1           | 10 |
| 14  | XN    | 49/50 (98%)    | 42 (86%)  | 7 (14%)  | 3           | 21 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 15  | QO    | 79/80 (99%)    | 72 (91%)  | 7 (9%)   | 9           | 40  |
| 15  | XO    | 79/80 (99%)    | 69 (87%)  | 10 (13%) | 4           | 24  |
| 16  | QP    | 72/74 (97%)    | 63 (88%)  | 9 (12%)  | 4           | 25  |
| 16  | XP    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 6           | 31  |
| 17  | QQ    | 95/97 (98%)    | 87 (92%)  | 8 (8%)   | 11          | 42  |
| 17  | XQ    | 95/97 (98%)    | 89 (94%)  | 6 (6%)   | 18          | 53  |
| 18  | QR    | 61/77 (79%)    | 50 (82%)  | 11 (18%) | 1           | 11  |
| 18  | XR    | 61/77 (79%)    | 52 (85%)  | 9 (15%)  | 3           | 19  |
| 19  | QS    | 73/80 (91%)    | 59 (81%)  | 14 (19%) | 1           | 9   |
| 19  | XS    | 73/80 (91%)    | 57 (78%)  | 16 (22%) | 1           | 6   |
| 20  | QT    | 76/82 (93%)    | 67 (88%)  | 9 (12%)  | 5           | 28  |
| 20  | XT    | 76/82 (93%)    | 66 (87%)  | 10 (13%) | 4           | 23  |
| 21  | QU    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 21  | XU    | 20/22 (91%)    | 19 (95%)  | 1 (5%)   | 24          | 59  |
| 27  | RD    | 214/218 (98%)  | 176 (82%) | 38 (18%) | 2           | 11  |
| 27  | YD    | 214/218 (98%)  | 180 (84%) | 34 (16%) | 2           | 16  |
| 28  | RE    | 165/166 (99%)  | 126 (76%) | 39 (24%) | 1           | 5   |
| 28  | YE    | 165/166 (99%)  | 135 (82%) | 30 (18%) | 1           | 10  |
| 29  | RF    | 161/166 (97%)  | 132 (82%) | 29 (18%) | 1           | 11  |
| 29  | YF    | 161/166 (97%)  | 137 (85%) | 24 (15%) | 3           | 19  |
| 30  | RG    | 155/156 (99%)  | 134 (86%) | 21 (14%) | 4           | 23  |
| 30  | YG    | 155/156 (99%)  | 134 (86%) | 21 (14%) | 4           | 23  |
| 31  | RH    | 142/148 (96%)  | 120 (84%) | 22 (16%) | 2           | 18  |
| 31  | YH    | 142/148 (96%)  | 116 (82%) | 26 (18%) | 1           | 10  |
| 32  | RI    | 122/124 (98%)  | 98 (80%)  | 24 (20%) | 1           | 8   |
| 32  | YI    | 122/124 (98%)  | 92 (75%)  | 30 (25%) | 0           | 4   |
| 33  | RN    | 117/119 (98%)  | 97 (83%)  | 20 (17%) | 2           | 13  |
| 33  | YN    | 117/119 (98%)  | 96 (82%)  | 21 (18%) | 2           | 11  |
| 34  | RO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 7           | 35  |
| 34  | YO    | 100/100 (100%) | 89 (89%)  | 11 (11%) | 6           | 31  |
| 35  | RP    | 116/116 (100%) | 86 (74%)  | 30 (26%) | 0           | 4   |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 35  | YP    | 116/116 (100%) | 81 (70%)  | 35 (30%) | 0           | 2  |
| 36  | RQ    | 111/111 (100%) | 94 (85%)  | 17 (15%) | 2           | 18 |
| 36  | YQ    | 111/111 (100%) | 92 (83%)  | 19 (17%) | 2           | 13 |
| 37  | RR    | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 11 |
| 37  | YR    | 101/101 (100%) | 80 (79%)  | 21 (21%) | 1           | 7  |
| 38  | RS    | 87/88 (99%)    | 69 (79%)  | 18 (21%) | 1           | 7  |
| 38  | YS    | 87/88 (99%)    | 68 (78%)  | 19 (22%) | 1           | 6  |
| 39  | RT    | 120/127 (94%)  | 102 (85%) | 18 (15%) | 3           | 19 |
| 39  | YT    | 120/127 (94%)  | 98 (82%)  | 22 (18%) | 1           | 10 |
| 40  | RU    | 93/94 (99%)    | 79 (85%)  | 14 (15%) | 3           | 19 |
| 40  | YU    | 93/94 (99%)    | 77 (83%)  | 16 (17%) | 2           | 13 |
| 41  | RV    | 82/82 (100%)   | 66 (80%)  | 16 (20%) | 1           | 9  |
| 41  | YV    | 82/82 (100%)   | 67 (82%)  | 15 (18%) | 1           | 10 |
| 42  | RW    | 92/92 (100%)   | 73 (79%)  | 19 (21%) | 1           | 7  |
| 42  | YW    | 92/92 (100%)   | 75 (82%)  | 17 (18%) | 1           | 10 |
| 43  | RX    | 74/78 (95%)    | 63 (85%)  | 11 (15%) | 3           | 19 |
| 43  | YX    | 74/78 (95%)    | 60 (81%)  | 14 (19%) | 1           | 9  |
| 44  | RY    | 85/91 (93%)    | 63 (74%)  | 22 (26%) | 0           | 4  |
| 44  | YY    | 85/91 (93%)    | 64 (75%)  | 21 (25%) | 0           | 4  |
| 45  | RZ    | 162/179 (90%)  | 132 (82%) | 30 (18%) | 1           | 10 |
| 45  | YZ    | 162/179 (90%)  | 133 (82%) | 29 (18%) | 2           | 11 |
| 46  | R0    | 65/67 (97%)    | 60 (92%)  | 5 (8%)   | 13          | 45 |
| 46  | Y0    | 65/67 (97%)    | 59 (91%)  | 6 (9%)   | 9           | 39 |
| 47  | R1    | 82/83 (99%)    | 73 (89%)  | 9 (11%)  | 6           | 31 |
| 47  | Y1    | 82/83 (99%)    | 70 (85%)  | 12 (15%) | 3           | 20 |
| 48  | R2    | 64/67 (96%)    | 57 (89%)  | 7 (11%)  | 6           | 32 |
| 48  | Y2    | 64/67 (96%)    | 47 (73%)  | 17 (27%) | 0           | 3  |
| 49  | R3    | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 5           | 28 |
| 49  | Y3    | 51/52 (98%)    | 43 (84%)  | 8 (16%)  | 2           | 17 |
| 50  | R4    | 63/63 (100%)   | 45 (71%)  | 18 (29%) | 0           | 3  |
| 50  | Y4    | 63/63 (100%)   | 43 (68%)  | 20 (32%) | 0           | 2  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|------------------|------------|------------|-------------|-----|
| 51  | R5    | 51/52 (98%)      | 36 (71%)   | 15 (29%)   | 0           | 2   |
| 51  | Y5    | 49/52 (94%)      | 36 (74%)   | 13 (26%)   | 0           | 3   |
| 52  | R6    | 48/52 (92%)      | 35 (73%)   | 13 (27%)   | 0           | 3   |
| 52  | Y6    | 48/52 (92%)      | 38 (79%)   | 10 (21%)   | 1           | 7   |
| 53  | R7    | 42/42 (100%)     | 34 (81%)   | 8 (19%)    | 1           | 9   |
| 53  | Y7    | 42/42 (100%)     | 35 (83%)   | 7 (17%)    | 2           | 14  |
| 54  | R8    | 54/55 (98%)      | 44 (82%)   | 10 (18%)   | 1           | 10  |
| 54  | Y8    | 54/55 (98%)      | 41 (76%)   | 13 (24%)   | 0           | 4   |
| 55  | R9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 19          | 55  |
| 55  | Y9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 19          | 55  |
| 56  | Z7    | 5/7 (71%)        | 5 (100%)   | 0          | 100         | 100 |
| 56  | Z8    | 5/7 (71%)        | 4 (80%)    | 1 (20%)    | 1           | 8   |
| All | All   | 9710/10080 (96%) | 8152 (84%) | 1558 (16%) | 2           | 16  |

All (1558) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 5   | ILE  |
| 2   | QB    | 6   | THR  |
| 2   | QB    | 7   | VAL  |
| 2   | QB    | 8   | LYS  |
| 2   | QB    | 15  | VAL  |
| 2   | QB    | 23  | ARG  |
| 2   | QB    | 24  | TRP  |
| 2   | QB    | 32  | ILE  |
| 2   | QB    | 33  | TYR  |
| 2   | QB    | 36  | ARG  |
| 2   | QB    | 53  | ARG  |
| 2   | QB    | 60  | ASP  |
| 2   | QB    | 67  | THR  |
| 2   | QB    | 82  | ARG  |
| 2   | QB    | 87  | ARG  |
| 2   | QB    | 92  | TYR  |
| 2   | QB    | 94  | ASN  |
| 2   | QB    | 101 | MET  |
| 2   | QB    | 109 | SER  |
| 2   | QB    | 119 | GLU  |
| 2   | QB    | 121 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 150 | SER  |
| 2   | QB    | 155 | LEU  |
| 2   | QB    | 158 | LEU  |
| 2   | QB    | 163 | PHE  |
| 2   | QB    | 165 | VAL  |
| 2   | QB    | 168 | THR  |
| 2   | QB    | 172 | ILE  |
| 2   | QB    | 175 | ARG  |
| 2   | QB    | 187 | LEU  |
| 2   | QB    | 196 | LEU  |
| 2   | QB    | 204 | ASN  |
| 2   | QB    | 215 | LEU  |
| 2   | QB    | 217 | ARG  |
| 3   | QC    | 3   | ASN  |
| 3   | QC    | 5   | ILE  |
| 3   | QC    | 12  | LEU  |
| 3   | QC    | 16  | ARG  |
| 3   | QC    | 21  | ARG  |
| 3   | QC    | 45  | LYS  |
| 3   | QC    | 52  | LEU  |
| 3   | QC    | 76  | VAL  |
| 3   | QC    | 94  | LEU  |
| 3   | QC    | 127 | ARG  |
| 3   | QC    | 131 | ARG  |
| 3   | QC    | 154 | SER  |
| 3   | QC    | 165 | THR  |
| 3   | QC    | 206 | GLU  |
| 4   | QD    | 3   | ARG  |
| 4   | QD    | 14  | ARG  |
| 4   | QD    | 22  | LYS  |
| 4   | QD    | 26  | CYS  |
| 4   | QD    | 30  | LYS  |
| 4   | QD    | 33  | MET  |
| 4   | QD    | 50  | ARG  |
| 4   | QD    | 58  | LEU  |
| 4   | QD    | 73  | ARG  |
| 4   | QD    | 76  | ARG  |
| 4   | QD    | 86  | LYS  |
| 4   | QD    | 94  | LEU  |
| 4   | QD    | 96  | LEU  |
| 4   | QD    | 122 | ARG  |
| 4   | QD    | 127 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | QD    | 131 | ARG  |
| 4   | QD    | 135 | LEU  |
| 4   | QD    | 154 | ASN  |
| 4   | QD    | 175 | SER  |
| 4   | QD    | 187 | ARG  |
| 4   | QD    | 190 | ASP  |
| 4   | QD    | 191 | ARG  |
| 4   | QD    | 192 | GLU  |
| 5   | QE    | 10  | MET  |
| 5   | QE    | 12  | LEU  |
| 5   | QE    | 31  | LEU  |
| 5   | QE    | 34  | VAL  |
| 5   | QE    | 41  | VAL  |
| 5   | QE    | 51  | VAL  |
| 5   | QE    | 68  | GLU  |
| 5   | QE    | 79  | GLU  |
| 5   | QE    | 81  | GLU  |
| 5   | QE    | 98  | THR  |
| 5   | QE    | 101 | ILE  |
| 5   | QE    | 153 | LYS  |
| 6   | QF    | 16  | GLN  |
| 6   | QF    | 21  | LEU  |
| 6   | QF    | 23  | LYS  |
| 6   | QF    | 43  | LEU  |
| 6   | QF    | 45  | LEU  |
| 6   | QF    | 47  | ARG  |
| 6   | QF    | 55  | ASP  |
| 6   | QF    | 69  | GLU  |
| 6   | QF    | 70  | ASP  |
| 6   | QF    | 72  | VAL  |
| 6   | QF    | 75  | LEU  |
| 6   | QF    | 98  | LEU  |
| 7   | QG    | 8   | GLU  |
| 7   | QG    | 54  | THR  |
| 7   | QG    | 80  | VAL  |
| 7   | QG    | 92  | SER  |
| 7   | QG    | 94  | ARG  |
| 7   | QG    | 104 | LEU  |
| 7   | QG    | 113 | GLU  |
| 7   | QG    | 114 | ARG  |
| 7   | QG    | 135 | VAL  |
| 7   | QG    | 136 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | QG    | 137 | LYS  |
| 7   | QG    | 155 | ARG  |
| 8   | QH    | 1   | MET  |
| 8   | QH    | 24  | THR  |
| 8   | QH    | 25  | ASP  |
| 8   | QH    | 26  | VAL  |
| 8   | QH    | 41  | ARG  |
| 8   | QH    | 99  | GLU  |
| 8   | QH    | 109 | ILE  |
| 8   | QH    | 112 | LEU  |
| 8   | QH    | 125 | ARG  |
| 8   | QH    | 129 | VAL  |
| 9   | QI    | 9   | ARG  |
| 9   | QI    | 10  | ARG  |
| 9   | QI    | 11  | LYS  |
| 9   | QI    | 23  | ASN  |
| 9   | QI    | 47  | LEU  |
| 9   | QI    | 56  | LEU  |
| 9   | QI    | 64  | THR  |
| 9   | QI    | 65  | VAL  |
| 9   | QI    | 75  | ASP  |
| 9   | QI    | 95  | LYS  |
| 9   | QI    | 104 | ARG  |
| 9   | QI    | 105 | ASP  |
| 9   | QI    | 113 | LYS  |
| 9   | QI    | 114 | TYR  |
| 9   | QI    | 121 | ARG  |
| 9   | QI    | 125 | TYR  |
| 9   | QI    | 128 | ARG  |
| 10  | QJ    | 22  | LYS  |
| 10  | QJ    | 47  | PHE  |
| 10  | QJ    | 54  | PHE  |
| 10  | QJ    | 57  | LYS  |
| 10  | QJ    | 58  | ASP  |
| 10  | QJ    | 62  | HIS  |
| 10  | QJ    | 73  | ASP  |
| 10  | QJ    | 74  | ILE  |
| 10  | QJ    | 80  | LYS  |
| 10  | QJ    | 84  | GLN  |
| 10  | QJ    | 92  | THR  |
| 10  | QJ    | 96  | ILE  |
| 11  | QK    | 26  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | QK    | 29  | ILE  |
| 11  | QK    | 32  | ILE  |
| 11  | QK    | 34  | ASP  |
| 11  | QK    | 63  | LEU  |
| 11  | QK    | 92  | GLU  |
| 11  | QK    | 103 | LEU  |
| 11  | QK    | 109 | VAL  |
| 11  | QK    | 127 | LYS  |
| 12  | QL    | 17  | LYS  |
| 12  | QL    | 18  | VAL  |
| 12  | QL    | 20  | LYS  |
| 12  | QL    | 27  | LEU  |
| 12  | QL    | 33  | ARG  |
| 12  | QL    | 38  | THR  |
| 12  | QL    | 42  | THR  |
| 12  | QL    | 50  | SER  |
| 12  | QL    | 54  | LYS  |
| 12  | QL    | 59  | ARG  |
| 12  | QL    | 60  | LEU  |
| 12  | QL    | 73  | GLU  |
| 12  | QL    | 83  | VAL  |
| 12  | QL    | 85  | ILE  |
| 12  | QL    | 89  | ARG  |
| 12  | QL    | 102 | ARG  |
| 12  | QL    | 113 | ARG  |
| 13  | QM    | 8   | GLU  |
| 13  | QM    | 11  | ARG  |
| 13  | QM    | 13  | LYS  |
| 13  | QM    | 17  | VAL  |
| 13  | QM    | 19  | LEU  |
| 13  | QM    | 45  | VAL  |
| 13  | QM    | 47  | ASP  |
| 13  | QM    | 48  | LEU  |
| 13  | QM    | 56  | LEU  |
| 13  | QM    | 57  | ARG  |
| 13  | QM    | 64  | TRP  |
| 13  | QM    | 66  | LEU  |
| 13  | QM    | 70  | LEU  |
| 13  | QM    | 77  | ASN  |
| 13  | QM    | 84  | ILE  |
| 13  | QM    | 88  | ARG  |
| 13  | QM    | 90  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | QM    | 98  | VAL  |
| 13  | QM    | 108 | ARG  |
| 13  | QM    | 111 | LYS  |
| 13  | QM    | 114 | ARG  |
| 13  | QM    | 115 | LYS  |
| 13  | QM    | 117 | VAL  |
| 13  | QM    | 122 | LYS  |
| 14  | QN    | 6   | LEU  |
| 14  | QN    | 12  | ARG  |
| 14  | QN    | 13  | THR  |
| 14  | QN    | 18  | VAL  |
| 14  | QN    | 33  | VAL  |
| 14  | QN    | 43  | CYS  |
| 14  | QN    | 44  | LEU  |
| 14  | QN    | 46  | GLU  |
| 14  | QN    | 57  | ARG  |
| 15  | QO    | 3   | ILE  |
| 15  | QO    | 4   | THR  |
| 15  | QO    | 26  | GLU  |
| 15  | QO    | 31  | LEU  |
| 15  | QO    | 39  | LEU  |
| 15  | QO    | 64  | ARG  |
| 15  | QO    | 84  | LYS  |
| 16  | QP    | 2   | VAL  |
| 16  | QP    | 20  | VAL  |
| 16  | QP    | 26  | ARG  |
| 16  | QP    | 28  | ARG  |
| 16  | QP    | 33  | ILE  |
| 16  | QP    | 53  | VAL  |
| 16  | QP    | 67  | THR  |
| 16  | QP    | 69  | THR  |
| 16  | QP    | 71  | ARG  |
| 17  | QQ    | 37  | LYS  |
| 17  | QQ    | 38  | ARG  |
| 17  | QQ    | 52  | LYS  |
| 17  | QQ    | 59  | ILE  |
| 17  | QQ    | 62  | SER  |
| 17  | QQ    | 68  | ARG  |
| 17  | QQ    | 74  | LEU  |
| 17  | QQ    | 101 | ARG  |
| 18  | QR    | 26  | LEU  |
| 18  | QR    | 29  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | QR    | 31  | LEU  |
| 18  | QR    | 32  | ARG  |
| 18  | QR    | 36  | ASN  |
| 18  | QR    | 46  | GLU  |
| 18  | QR    | 54  | ARG  |
| 18  | QR    | 76  | LEU  |
| 18  | QR    | 82  | THR  |
| 18  | QR    | 83  | GLU  |
| 18  | QR    | 86  | VAL  |
| 19  | QS    | 5   | LEU  |
| 19  | QS    | 10  | PHE  |
| 19  | QS    | 12  | ASP  |
| 19  | QS    | 21  | GLU  |
| 19  | QS    | 28  | LYS  |
| 19  | QS    | 29  | ARG  |
| 19  | QS    | 30  | LEU  |
| 19  | QS    | 37  | ARG  |
| 19  | QS    | 43  | GLU  |
| 19  | QS    | 44  | MET  |
| 19  | QS    | 63  | THR  |
| 19  | QS    | 67  | VAL  |
| 19  | QS    | 77  | THR  |
| 19  | QS    | 83  | HIS  |
| 20  | QT    | 17  | ARG  |
| 20  | QT    | 24  | LEU  |
| 20  | QT    | 45  | GLN  |
| 20  | QT    | 72  | LEU  |
| 20  | QT    | 73  | HIS  |
| 20  | QT    | 75  | ASN  |
| 20  | QT    | 80  | ARG  |
| 20  | QT    | 84  | LEU  |
| 20  | QT    | 93  | GLU  |
| 27  | RD    | 10  | THR  |
| 27  | RD    | 17  | THR  |
| 27  | RD    | 25  | THR  |
| 27  | RD    | 40  | THR  |
| 27  | RD    | 43  | ARG  |
| 27  | RD    | 44  | ASN  |
| 27  | RD    | 46  | GLN  |
| 27  | RD    | 49  | ILE  |
| 27  | RD    | 61  | LEU  |
| 27  | RD    | 65  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | RD    | 69  | ARG  |
| 27  | RD    | 71  | ASP  |
| 27  | RD    | 73  | VAL  |
| 27  | RD    | 83  | GLU  |
| 27  | RD    | 87  | ASN  |
| 27  | RD    | 88  | ARG  |
| 27  | RD    | 95  | LEU  |
| 27  | RD    | 103 | ARG  |
| 27  | RD    | 105 | ILE  |
| 27  | RD    | 106 | ILE  |
| 27  | RD    | 111 | LEU  |
| 27  | RD    | 150 | LYS  |
| 27  | RD    | 155 | LEU  |
| 27  | RD    | 157 | ARG  |
| 27  | RD    | 173 | VAL  |
| 27  | RD    | 192 | THR  |
| 27  | RD    | 211 | ARG  |
| 27  | RD    | 212 | SER  |
| 27  | RD    | 221 | VAL  |
| 27  | RD    | 229 | VAL  |
| 27  | RD    | 237 | GLU  |
| 27  | RD    | 242 | ARG  |
| 27  | RD    | 257 | LEU  |
| 27  | RD    | 259 | THR  |
| 27  | RD    | 261 | LYS  |
| 27  | RD    | 268 | ARG  |
| 27  | RD    | 271 | ILE  |
| 27  | RD    | 273 | ARG  |
| 28  | RE    | 2   | LYS  |
| 28  | RE    | 4   | ILE  |
| 28  | RE    | 7   | VAL  |
| 28  | RE    | 12  | THR  |
| 28  | RE    | 13  | ARG  |
| 28  | RE    | 16  | ARG  |
| 28  | RE    | 26  | ILE  |
| 28  | RE    | 27  | LEU  |
| 28  | RE    | 33  | VAL  |
| 28  | RE    | 34  | VAL  |
| 28  | RE    | 38  | THR  |
| 28  | RE    | 41  | LYS  |
| 28  | RE    | 42  | ASP  |
| 28  | RE    | 47  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | RE    | 49  | LEU  |
| 28  | RE    | 52  | LEU  |
| 28  | RE    | 54  | GLN  |
| 28  | RE    | 63  | LEU  |
| 28  | RE    | 77  | ILE  |
| 28  | RE    | 79  | ARG  |
| 28  | RE    | 80  | GLU  |
| 28  | RE    | 82  | ARG  |
| 28  | RE    | 92  | THR  |
| 28  | RE    | 101 | ARG  |
| 28  | RE    | 113 | PHE  |
| 28  | RE    | 116 | VAL  |
| 28  | RE    | 119 | ARG  |
| 28  | RE    | 127 | ASP  |
| 28  | RE    | 144 | ARG  |
| 28  | RE    | 146 | THR  |
| 28  | RE    | 167 | VAL  |
| 28  | RE    | 175 | VAL  |
| 28  | RE    | 179 | GLU  |
| 28  | RE    | 181 | LEU  |
| 28  | RE    | 184 | VAL  |
| 28  | RE    | 197 | ILE  |
| 28  | RE    | 200 | GLU  |
| 28  | RE    | 202 | LYS  |
| 28  | RE    | 203 | LYS  |
| 29  | RF    | 9   | ILE  |
| 29  | RF    | 13  | SER  |
| 29  | RF    | 24  | LEU  |
| 29  | RF    | 28  | ILE  |
| 29  | RF    | 32  | LEU  |
| 29  | RF    | 33  | LEU  |
| 29  | RF    | 45  | ARG  |
| 29  | RF    | 57  | VAL  |
| 29  | RF    | 65  | TRP  |
| 29  | RF    | 68  | LYS  |
| 29  | RF    | 70  | THR  |
| 29  | RF    | 74  | ARG  |
| 29  | RF    | 77  | ASP  |
| 29  | RF    | 78  | ILE  |
| 29  | RF    | 84  | VAL  |
| 29  | RF    | 104 | LYS  |
| 29  | RF    | 107 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | RF    | 117 | ARG  |
| 29  | RF    | 127 | GLU  |
| 29  | RF    | 149 | ASP  |
| 29  | RF    | 158 | THR  |
| 29  | RF    | 161 | GLU  |
| 29  | RF    | 165 | ARG  |
| 29  | RF    | 174 | VAL  |
| 29  | RF    | 176 | LEU  |
| 29  | RF    | 181 | LEU  |
| 29  | RF    | 192 | LEU  |
| 29  | RF    | 194 | MET  |
| 29  | RF    | 197 | ASP  |
| 30  | RG    | 7   | LEU  |
| 30  | RG    | 10  | LYS  |
| 30  | RG    | 20  | ILE  |
| 30  | RG    | 26  | GLN  |
| 30  | RG    | 33  | ARG  |
| 30  | RG    | 34  | LEU  |
| 30  | RG    | 43  | LEU  |
| 30  | RG    | 53  | LEU  |
| 30  | RG    | 54  | GLU  |
| 30  | RG    | 67  | LYS  |
| 30  | RG    | 71  | THR  |
| 30  | RG    | 88  | ILE  |
| 30  | RG    | 94  | LEU  |
| 30  | RG    | 98  | ARG  |
| 30  | RG    | 116 | ASP  |
| 30  | RG    | 118 | ARG  |
| 30  | RG    | 133 | LEU  |
| 30  | RG    | 147 | ASP  |
| 30  | RG    | 159 | VAL  |
| 30  | RG    | 167 | GLU  |
| 30  | RG    | 174 | GLU  |
| 31  | RH    | 3   | ARG  |
| 31  | RH    | 4   | ILE  |
| 31  | RH    | 7   | LEU  |
| 31  | RH    | 9   | ILE  |
| 31  | RH    | 27  | LYS  |
| 31  | RH    | 42  | ARG  |
| 31  | RH    | 43  | VAL  |
| 31  | RH    | 51  | ARG  |
| 31  | RH    | 59  | ARG  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 31         | RH           | 64         | LEU         |
| 31         | RH           | 77         | LYS         |
| 31         | RH           | 81         | GLU         |
| 31         | RH           | 88         | LEU         |
| 31         | RH           | 89         | ILE         |
| 31         | RH           | 105        | LEU         |
| 31         | RH           | 107        | VAL         |
| 31         | RH           | 127        | GLU         |
| 31         | RH           | 132        | ARG         |
| 31         | RH           | 152        | ARG         |
| 31         | RH           | 153        | LYS         |
| 31         | RH           | 158        | HIS         |
| 31         | RH           | 169        | VAL         |
| 32         | RI           | 1          | MET         |
| 32         | RI           | 2          | LYS         |
| 32         | RI           | 9          | LEU         |
| 32         | RI           | 10         | GLU         |
| 32         | RI           | 27         | ARG         |
| 32         | RI           | 31         | LEU         |
| 32         | RI           | 33         | ARG         |
| 32         | RI           | 38         | LEU         |
| 32         | RI           | 44         | LEU         |
| 32         | RI           | 56         | LYS         |
| 32         | RI           | 57         | ARG         |
| 32         | RI           | 70         | GLU         |
| 32         | RI           | 72         | LEU         |
| 32         | RI           | 81         | VAL         |
| 32         | RI           | 92         | VAL         |
| 32         | RI           | 101        | LEU         |
| 32         | RI           | 113        | ARG         |
| 32         | RI           | 128        | LEU         |
| 32         | RI           | 129        | THR         |
| 32         | RI           | 130        | TYR         |
| 32         | RI           | 131        | LYS         |
| 32         | RI           | 135        | GLU         |
| 32         | RI           | 142        | VAL         |
| 32         | RI           | 145        | VAL         |
| 33         | RN           | 1          | MET         |
| 33         | RN           | 2          | LYS         |
| 33         | RN           | 5          | VAL         |
| 33         | RN           | 7          | LYS         |
| 33         | RN           | 12         | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 33         | RN           | 32         | THR         |
| 33         | RN           | 34         | LEU         |
| 33         | RN           | 43         | THR         |
| 33         | RN           | 48         | MET         |
| 33         | RN           | 60         | ILE         |
| 33         | RN           | 61         | ARG         |
| 33         | RN           | 62         | VAL         |
| 33         | RN           | 87         | LEU         |
| 33         | RN           | 90         | MET         |
| 33         | RN           | 96         | GLU         |
| 33         | RN           | 98         | VAL         |
| 33         | RN           | 109        | LYS         |
| 33         | RN           | 120        | LEU         |
| 33         | RN           | 127        | ASP         |
| 33         | RN           | 136        | GLU         |
| 34         | RO           | 3          | GLN         |
| 34         | RO           | 9          | GLU         |
| 34         | RO           | 19         | ILE         |
| 34         | RO           | 24         | VAL         |
| 34         | RO           | 31         | LYS         |
| 34         | RO           | 49         | ARG         |
| 34         | RO           | 53         | LYS         |
| 34         | RO           | 69         | ILE         |
| 34         | RO           | 91         | LEU         |
| 34         | RO           | 102        | VAL         |
| 35         | RP           | 5          | ASP         |
| 35         | RP           | 6          | LEU         |
| 35         | RP           | 14         | LYS         |
| 35         | RP           | 15         | ARG         |
| 35         | RP           | 16         | ARG         |
| 35         | RP           | 19         | VAL         |
| 35         | RP           | 21         | ARG         |
| 35         | RP           | 30         | THR         |
| 35         | RP           | 36         | LYS         |
| 35         | RP           | 41         | ARG         |
| 35         | RP           | 45         | LEU         |
| 35         | RP           | 50         | ARG         |
| 35         | RP           | 56         | SER         |
| 35         | RP           | 61         | ARG         |
| 35         | RP           | 62         | LEU         |
| 35         | RP           | 64         | LYS         |
| 35         | RP           | 70         | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | RP    | 71  | VAL  |
| 35  | RP    | 75  | ILE  |
| 35  | RP    | 81  | GLN  |
| 35  | RP    | 88  | LEU  |
| 35  | RP    | 91  | PHE  |
| 35  | RP    | 100 | LEU  |
| 35  | RP    | 105 | LEU  |
| 35  | RP    | 107 | LYS  |
| 35  | RP    | 112 | LEU  |
| 35  | RP    | 133 | SER  |
| 35  | RP    | 138 | LEU  |
| 35  | RP    | 144 | GLU  |
| 35  | RP    | 146 | VAL  |
| 36  | RQ    | 17  | LEU  |
| 36  | RQ    | 26  | TYR  |
| 36  | RQ    | 27  | VAL  |
| 36  | RQ    | 35  | VAL  |
| 36  | RQ    | 45  | GLN  |
| 36  | RQ    | 54  | MET  |
| 36  | RQ    | 60  | ARG  |
| 36  | RQ    | 79  | LEU  |
| 36  | RQ    | 80  | GLU  |
| 36  | RQ    | 81  | VAL  |
| 36  | RQ    | 82  | ARG  |
| 36  | RQ    | 83  | MET  |
| 36  | RQ    | 85  | LYS  |
| 36  | RQ    | 96  | VAL  |
| 36  | RQ    | 112 | GLU  |
| 36  | RQ    | 135 | ASP  |
| 36  | RQ    | 139 | GLU  |
| 37  | RR    | 1   | MET  |
| 37  | RR    | 6   | SER  |
| 37  | RR    | 9   | LYS  |
| 37  | RR    | 18  | LEU  |
| 37  | RR    | 29  | LEU  |
| 37  | RR    | 35  | THR  |
| 37  | RR    | 44  | LEU  |
| 37  | RR    | 63  | ARG  |
| 37  | RR    | 71  | GLN  |
| 37  | RR    | 75  | LEU  |
| 37  | RR    | 79  | LEU  |
| 37  | RR    | 91  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | RR    | 95  | THR  |
| 37  | RR    | 100 | LEU  |
| 37  | RR    | 104 | ARG  |
| 37  | RR    | 105 | ARG  |
| 37  | RR    | 117 | VAL  |
| 37  | RR    | 118 | GLU  |
| 38  | RS    | 3   | ARG  |
| 38  | RS    | 4   | LEU  |
| 38  | RS    | 12  | PHE  |
| 38  | RS    | 17  | ARG  |
| 38  | RS    | 20  | ARG  |
| 38  | RS    | 27  | SER  |
| 38  | RS    | 39  | ILE  |
| 38  | RS    | 44  | LYS  |
| 38  | RS    | 50  | SER  |
| 38  | RS    | 54  | LEU  |
| 38  | RS    | 56  | LEU  |
| 38  | RS    | 57  | LYS  |
| 38  | RS    | 58  | LEU  |
| 38  | RS    | 59  | LYS  |
| 38  | RS    | 98  | VAL  |
| 38  | RS    | 101 | LEU  |
| 38  | RS    | 103 | GLU  |
| 38  | RS    | 106 | ARG  |
| 39  | RT    | 18  | ASP  |
| 39  | RT    | 27  | THR  |
| 39  | RT    | 30  | VAL  |
| 39  | RT    | 41  | ARG  |
| 39  | RT    | 42  | ILE  |
| 39  | RT    | 50  | ILE  |
| 39  | RT    | 51  | ARG  |
| 39  | RT    | 62  | THR  |
| 39  | RT    | 65  | LYS  |
| 39  | RT    | 74  | ARG  |
| 39  | RT    | 88  | ILE  |
| 39  | RT    | 89  | VAL  |
| 39  | RT    | 99  | LEU  |
| 39  | RT    | 105 | LEU  |
| 39  | RT    | 107 | ASP  |
| 39  | RT    | 112 | ARG  |
| 39  | RT    | 125 | ARG  |
| 39  | RT    | 128 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | RU    | 52  | ARG  |
| 40  | RU    | 55  | ARG  |
| 40  | RU    | 59  | ARG  |
| 40  | RU    | 60  | LEU  |
| 40  | RU    | 64  | ARG  |
| 40  | RU    | 69  | CYS  |
| 40  | RU    | 74  | LEU  |
| 40  | RU    | 90  | VAL  |
| 40  | RU    | 92  | ARG  |
| 40  | RU    | 98  | LEU  |
| 40  | RU    | 108 | GLU  |
| 40  | RU    | 111 | GLU  |
| 40  | RU    | 114 | LYS  |
| 40  | RU    | 117 | GLN  |
| 41  | RV    | 13  | ARG  |
| 41  | RV    | 19  | LYS  |
| 41  | RV    | 21  | ARG  |
| 41  | RV    | 22  | VAL  |
| 41  | RV    | 24  | LYS  |
| 41  | RV    | 35  | LEU  |
| 41  | RV    | 37  | VAL  |
| 41  | RV    | 45  | THR  |
| 41  | RV    | 47  | VAL  |
| 41  | RV    | 57  | VAL  |
| 41  | RV    | 61  | VAL  |
| 41  | RV    | 62  | LEU  |
| 41  | RV    | 64  | HIS  |
| 41  | RV    | 78  | LYS  |
| 41  | RV    | 79  | VAL  |
| 41  | RV    | 99  | ILE  |
| 42  | RW    | 11  | ARG  |
| 42  | RW    | 16  | LYS  |
| 42  | RW    | 18  | ARG  |
| 42  | RW    | 19  | LEU  |
| 42  | RW    | 20  | VAL  |
| 42  | RW    | 23  | LEU  |
| 42  | RW    | 27  | LYS  |
| 42  | RW    | 30  | GLU  |
| 42  | RW    | 40  | ASN  |
| 42  | RW    | 51  | LEU  |
| 42  | RW    | 60  | ASN  |
| 42  | RW    | 63  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | RW    | 67  | ASP  |
| 42  | RW    | 76  | VAL  |
| 42  | RW    | 82  | LEU  |
| 42  | RW    | 92  | ARG  |
| 42  | RW    | 100 | THR  |
| 42  | RW    | 106 | ILE  |
| 42  | RW    | 107 | LEU  |
| 43  | RX    | 12  | VAL  |
| 43  | RX    | 23  | GLU  |
| 43  | RX    | 27  | THR  |
| 43  | RX    | 30  | VAL  |
| 43  | RX    | 35  | THR  |
| 43  | RX    | 49  | VAL  |
| 43  | RX    | 55  | ASN  |
| 43  | RX    | 65  | ARG  |
| 43  | RX    | 70  | LEU  |
| 43  | RX    | 80  | ILE  |
| 43  | RX    | 81  | VAL  |
| 44  | RY    | 2   | ARG  |
| 44  | RY    | 13  | VAL  |
| 44  | RY    | 14  | LEU  |
| 44  | RY    | 27  | VAL  |
| 44  | RY    | 34  | LYS  |
| 44  | RY    | 37  | VAL  |
| 44  | RY    | 38  | ILE  |
| 44  | RY    | 43  | ASN  |
| 44  | RY    | 45  | VAL  |
| 44  | RY    | 55  | TYR  |
| 44  | RY    | 57  | GLN  |
| 44  | RY    | 61  | ILE  |
| 44  | RY    | 67  | LEU  |
| 44  | RY    | 70  | SER  |
| 44  | RY    | 75  | ILE  |
| 44  | RY    | 76  | CYS  |
| 44  | RY    | 87  | LYS  |
| 44  | RY    | 90  | LEU  |
| 44  | RY    | 95  | LYS  |
| 44  | RY    | 96  | ILE  |
| 44  | RY    | 97  | ARG  |
| 44  | RY    | 102 | CYS  |
| 45  | RZ    | 2   | GLU  |
| 45  | RZ    | 5   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | RZ    | 19  | ARG  |
| 45  | RZ    | 20  | ARG  |
| 45  | RZ    | 52  | SER  |
| 45  | RZ    | 53  | ILE  |
| 45  | RZ    | 60  | GLU  |
| 45  | RZ    | 70  | LEU  |
| 45  | RZ    | 71  | VAL  |
| 45  | RZ    | 81  | ARG  |
| 45  | RZ    | 87  | ASP  |
| 45  | RZ    | 91  | LEU  |
| 45  | RZ    | 92  | SER  |
| 45  | RZ    | 93  | ASP  |
| 45  | RZ    | 94  | GLU  |
| 45  | RZ    | 107 | THR  |
| 45  | RZ    | 112 | ARG  |
| 45  | RZ    | 117 | LEU  |
| 45  | RZ    | 121 | HIS  |
| 45  | RZ    | 128 | VAL  |
| 45  | RZ    | 131 | ARG  |
| 45  | RZ    | 142 | SER  |
| 45  | RZ    | 145 | GLU  |
| 45  | RZ    | 150 | LEU  |
| 45  | RZ    | 151 | HIS  |
| 45  | RZ    | 163 | LEU  |
| 45  | RZ    | 168 | GLU  |
| 45  | RZ    | 174 | VAL  |
| 45  | RZ    | 182 | LYS  |
| 45  | RZ    | 183 | LEU  |
| 46  | R0    | 7   | LEU  |
| 46  | R0    | 10  | THR  |
| 46  | R0    | 36  | ILE  |
| 46  | R0    | 53  | MET  |
| 46  | R0    | 74  | ARG  |
| 47  | R1    | 21  | ARG  |
| 47  | R1    | 41  | ARG  |
| 47  | R1    | 51  | VAL  |
| 47  | R1    | 62  | VAL  |
| 47  | R1    | 78  | LYS  |
| 47  | R1    | 80  | LEU  |
| 47  | R1    | 90  | ILE  |
| 47  | R1    | 91  | LYS  |
| 47  | R1    | 92  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | R2    | 17  | SER  |
| 48  | R2    | 24  | LEU  |
| 48  | R2    | 27  | GLU  |
| 48  | R2    | 32  | LEU  |
| 48  | R2    | 50  | ILE  |
| 48  | R2    | 53  | LEU  |
| 48  | R2    | 62  | THR  |
| 49  | R3    | 6   | VAL  |
| 49  | R3    | 8   | LEU  |
| 49  | R3    | 18  | ASP  |
| 49  | R3    | 32  | GLN  |
| 49  | R3    | 40  | THR  |
| 49  | R3    | 56  | VAL  |
| 50  | R4    | 13  | ARG  |
| 50  | R4    | 15  | ILE  |
| 50  | R4    | 23  | GLU  |
| 50  | R4    | 33  | VAL  |
| 50  | R4    | 34  | GLU  |
| 50  | R4    | 37  | SER  |
| 50  | R4    | 42  | PHE  |
| 50  | R4    | 48  | ARG  |
| 50  | R4    | 49  | PHE  |
| 50  | R4    | 50  | VAL  |
| 50  | R4    | 52  | THR  |
| 50  | R4    | 57  | GLU  |
| 50  | R4    | 61  | ARG  |
| 50  | R4    | 62  | ARG  |
| 50  | R4    | 63  | TYR  |
| 50  | R4    | 66  | SER  |
| 50  | R4    | 67  | TYR  |
| 50  | R4    | 68  | ARG  |
| 51  | R5    | 4   | HIS  |
| 51  | R5    | 6   | VAL  |
| 51  | R5    | 11  | THR  |
| 51  | R5    | 21  | SER  |
| 51  | R5    | 23  | HIS  |
| 51  | R5    | 25  | LEU  |
| 51  | R5    | 29  | THR  |
| 51  | R5    | 36  | CYS  |
| 51  | R5    | 40  | LYS  |
| 51  | R5    | 46  | CYS  |
| 51  | R5    | 51  | TYR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 51         | R5           | 55         | ARG         |
| 51         | R5           | 56         | LYS         |
| 51         | R5           | 58         | LEU         |
| 51         | R5           | 60         | VAL         |
| 52         | R6           | 6          | ARG         |
| 52         | R6           | 8          | LYS         |
| 52         | R6           | 9          | LEU         |
| 52         | R6           | 10         | LEU         |
| 52         | R6           | 11         | LEU         |
| 52         | R6           | 17         | LYS         |
| 52         | R6           | 19         | ARG         |
| 52         | R6           | 23         | THR         |
| 52         | R6           | 27         | LYS         |
| 52         | R6           | 30         | THR         |
| 52         | R6           | 34         | LEU         |
| 52         | R6           | 37         | ARG         |
| 52         | R6           | 44         | ARG         |
| 53         | R7           | 1          | MET         |
| 53         | R7           | 2          | LYS         |
| 53         | R7           | 4          | THR         |
| 53         | R7           | 9          | ARG         |
| 53         | R7           | 10         | ARG         |
| 53         | R7           | 14         | LYS         |
| 53         | R7           | 43         | THR         |
| 53         | R7           | 46         | VAL         |
| 54         | R8           | 14         | VAL         |
| 54         | R8           | 15         | LYS         |
| 54         | R8           | 34         | TRP         |
| 54         | R8           | 35         | GLN         |
| 54         | R8           | 44         | LYS         |
| 54         | R8           | 47         | LYS         |
| 54         | R8           | 49         | VAL         |
| 54         | R8           | 52         | LYS         |
| 54         | R8           | 64         | TYR         |
| 54         | R8           | 65         | GLU         |
| 55         | R9           | 1          | MET         |
| 55         | R9           | 29         | ASN         |
| 2          | XB           | 5          | ILE         |
| 2          | XB           | 7          | VAL         |
| 2          | XB           | 8          | LYS         |
| 2          | XB           | 15         | VAL         |
| 2          | XB           | 23         | ARG         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | XB    | 24  | TRP  |
| 2   | XB    | 33  | TYR  |
| 2   | XB    | 36  | ARG  |
| 2   | XB    | 67  | THR  |
| 2   | XB    | 71  | VAL  |
| 2   | XB    | 82  | ARG  |
| 2   | XB    | 92  | TYR  |
| 2   | XB    | 113 | HIS  |
| 2   | XB    | 145 | LEU  |
| 2   | XB    | 155 | LEU  |
| 2   | XB    | 163 | PHE  |
| 2   | XB    | 172 | ILE  |
| 2   | XB    | 175 | ARG  |
| 2   | XB    | 178 | ARG  |
| 2   | XB    | 187 | LEU  |
| 2   | XB    | 195 | ASP  |
| 2   | XB    | 196 | LEU  |
| 2   | XB    | 204 | ASN  |
| 2   | XB    | 215 | LEU  |
| 2   | XB    | 235 | SER  |
| 3   | XC    | 3   | ASN  |
| 3   | XC    | 5   | ILE  |
| 3   | XC    | 12  | LEU  |
| 3   | XC    | 21  | ARG  |
| 3   | XC    | 45  | LYS  |
| 3   | XC    | 47  | LEU  |
| 3   | XC    | 56  | ASP  |
| 3   | XC    | 94  | LEU  |
| 3   | XC    | 95  | THR  |
| 3   | XC    | 131 | ARG  |
| 3   | XC    | 178 | LEU  |
| 3   | XC    | 184 | TYR  |
| 3   | XC    | 192 | THR  |
| 4   | XD    | 3   | ARG  |
| 4   | XD    | 9   | CYS  |
| 4   | XD    | 15  | GLU  |
| 4   | XD    | 19  | LEU  |
| 4   | XD    | 22  | LYS  |
| 4   | XD    | 26  | CYS  |
| 4   | XD    | 30  | LYS  |
| 4   | XD    | 33  | MET  |
| 4   | XD    | 50  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | XD    | 53  | ASP  |
| 4   | XD    | 58  | LEU  |
| 4   | XD    | 73  | ARG  |
| 4   | XD    | 76  | ARG  |
| 4   | XD    | 84  | LYS  |
| 4   | XD    | 86  | LYS  |
| 4   | XD    | 96  | LEU  |
| 4   | XD    | 108 | LEU  |
| 4   | XD    | 122 | ARG  |
| 4   | XD    | 127 | THR  |
| 4   | XD    | 131 | ARG  |
| 4   | XD    | 137 | SER  |
| 4   | XD    | 150 | GLU  |
| 4   | XD    | 154 | ASN  |
| 4   | XD    | 175 | SER  |
| 4   | XD    | 187 | ARG  |
| 4   | XD    | 190 | ASP  |
| 4   | XD    | 193 | ASP  |
| 4   | XD    | 208 | SER  |
| 5   | XE    | 6   | PHE  |
| 5   | XE    | 7   | GLU  |
| 5   | XE    | 10  | MET  |
| 5   | XE    | 11  | ILE  |
| 5   | XE    | 18  | ARG  |
| 5   | XE    | 31  | LEU  |
| 5   | XE    | 41  | VAL  |
| 5   | XE    | 73  | ASN  |
| 5   | XE    | 79  | GLU  |
| 5   | XE    | 101 | ILE  |
| 5   | XE    | 147 | ASP  |
| 5   | XE    | 153 | LYS  |
| 6   | XF    | 17  | SER  |
| 6   | XF    | 21  | LEU  |
| 6   | XF    | 23  | LYS  |
| 6   | XF    | 36  | ARG  |
| 6   | XF    | 71  | ARG  |
| 6   | XF    | 74  | ASP  |
| 6   | XF    | 91  | VAL  |
| 6   | XF    | 92  | LYS  |
| 6   | XF    | 98  | LEU  |
| 7   | XG    | 5   | ARG  |
| 7   | XG    | 8   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | XG    | 35  | LYS  |
| 7   | XG    | 54  | THR  |
| 7   | XG    | 63  | LYS  |
| 7   | XG    | 78  | ARG  |
| 7   | XG    | 104 | LEU  |
| 7   | XG    | 113 | GLU  |
| 7   | XG    | 114 | ARG  |
| 7   | XG    | 136 | LYS  |
| 7   | XG    | 137 | LYS  |
| 7   | XG    | 155 | ARG  |
| 8   | XH    | 1   | MET  |
| 8   | XH    | 12  | ARG  |
| 8   | XH    | 19  | VAL  |
| 8   | XH    | 24  | THR  |
| 8   | XH    | 26  | VAL  |
| 8   | XH    | 41  | ARG  |
| 8   | XH    | 54  | ASP  |
| 8   | XH    | 63  | LEU  |
| 8   | XH    | 80  | ILE  |
| 8   | XH    | 85  | ARG  |
| 8   | XH    | 109 | ILE  |
| 8   | XH    | 112 | LEU  |
| 8   | XH    | 137 | VAL  |
| 9   | XI    | 9   | ARG  |
| 9   | XI    | 38  | GLN  |
| 9   | XI    | 44  | VAL  |
| 9   | XI    | 56  | LEU  |
| 9   | XI    | 65  | VAL  |
| 9   | XI    | 95  | LYS  |
| 9   | XI    | 96  | LEU  |
| 9   | XI    | 102 | LEU  |
| 9   | XI    | 104 | ARG  |
| 9   | XI    | 105 | ASP  |
| 9   | XI    | 108 | VAL  |
| 9   | XI    | 111 | ARG  |
| 9   | XI    | 112 | LYS  |
| 9   | XI    | 114 | TYR  |
| 9   | XI    | 121 | ARG  |
| 9   | XI    | 124 | GLN  |
| 9   | XI    | 125 | TYR  |
| 9   | XI    | 128 | ARG  |
| 10  | XJ    | 3   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | XJ    | 17  | ASP  |
| 10  | XJ    | 22  | LYS  |
| 10  | XJ    | 45  | ARG  |
| 10  | XJ    | 47  | PHE  |
| 10  | XJ    | 49  | VAL  |
| 10  | XJ    | 54  | PHE  |
| 10  | XJ    | 57  | LYS  |
| 10  | XJ    | 62  | HIS  |
| 10  | XJ    | 70  | ARG  |
| 10  | XJ    | 74  | ILE  |
| 10  | XJ    | 80  | LYS  |
| 10  | XJ    | 84  | GLN  |
| 10  | XJ    | 96  | ILE  |
| 10  | XJ    | 98  | ILE  |
| 11  | XK    | 26  | ASN  |
| 11  | XK    | 29  | ILE  |
| 11  | XK    | 31  | THR  |
| 11  | XK    | 32  | ILE  |
| 11  | XK    | 36  | ASP  |
| 11  | XK    | 57  | THR  |
| 11  | XK    | 96  | ARG  |
| 11  | XK    | 114 | VAL  |
| 11  | XK    | 116 | HIS  |
| 12  | XL    | 17  | LYS  |
| 12  | XL    | 18  | VAL  |
| 12  | XL    | 20  | LYS  |
| 12  | XL    | 27  | LEU  |
| 12  | XL    | 33  | ARG  |
| 12  | XL    | 47  | LYS  |
| 12  | XL    | 59  | ARG  |
| 12  | XL    | 62  | SER  |
| 12  | XL    | 81  | SER  |
| 12  | XL    | 89  | ARG  |
| 12  | XL    | 91  | LYS  |
| 12  | XL    | 126 | LYS  |
| 13  | XM    | 3   | ARG  |
| 13  | XM    | 13  | LYS  |
| 13  | XM    | 17  | VAL  |
| 13  | XM    | 19  | LEU  |
| 13  | XM    | 32  | GLU  |
| 13  | XM    | 45  | VAL  |
| 13  | XM    | 48  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | XM    | 56  | LEU  |
| 13  | XM    | 64  | TRP  |
| 13  | XM    | 66  | LEU  |
| 13  | XM    | 70  | LEU  |
| 13  | XM    | 84  | ILE  |
| 13  | XM    | 88  | ARG  |
| 13  | XM    | 98  | VAL  |
| 13  | XM    | 108 | ARG  |
| 13  | XM    | 114 | ARG  |
| 13  | XM    | 115 | LYS  |
| 13  | XM    | 117 | VAL  |
| 13  | XM    | 122 | LYS  |
| 14  | XN    | 6   | LEU  |
| 14  | XN    | 12  | ARG  |
| 14  | XN    | 32  | SER  |
| 14  | XN    | 33  | VAL  |
| 14  | XN    | 40  | CYS  |
| 14  | XN    | 41  | ARG  |
| 14  | XN    | 44  | LEU  |
| 15  | XO    | 3   | ILE  |
| 15  | XO    | 8   | LYS  |
| 15  | XO    | 24  | SER  |
| 15  | XO    | 26  | GLU  |
| 15  | XO    | 39  | LEU  |
| 15  | XO    | 62  | GLN  |
| 15  | XO    | 64  | ARG  |
| 15  | XO    | 66  | LEU  |
| 15  | XO    | 82  | ILE  |
| 15  | XO    | 87  | ILE  |
| 16  | XP    | 2   | VAL  |
| 16  | XP    | 11  | SER  |
| 16  | XP    | 20  | VAL  |
| 16  | XP    | 28  | ARG  |
| 16  | XP    | 32  | TYR  |
| 16  | XP    | 67  | THR  |
| 16  | XP    | 69  | THR  |
| 16  | XP    | 72  | ARG  |
| 17  | XQ    | 52  | LYS  |
| 17  | XQ    | 59  | ILE  |
| 17  | XQ    | 62  | SER  |
| 17  | XQ    | 68  | ARG  |
| 17  | XQ    | 74  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | XQ    | 101 | ARG  |
| 18  | XR    | 26  | LEU  |
| 18  | XR    | 29  | PHE  |
| 18  | XR    | 36  | ASN  |
| 18  | XR    | 41  | LYS  |
| 18  | XR    | 46  | GLU  |
| 18  | XR    | 54  | ARG  |
| 18  | XR    | 76  | LEU  |
| 18  | XR    | 82  | THR  |
| 18  | XR    | 86  | VAL  |
| 19  | XS    | 5   | LEU  |
| 19  | XS    | 10  | PHE  |
| 19  | XS    | 11  | VAL  |
| 19  | XS    | 12  | ASP  |
| 19  | XS    | 13  | ASP  |
| 19  | XS    | 21  | GLU  |
| 19  | XS    | 28  | LYS  |
| 19  | XS    | 29  | ARG  |
| 19  | XS    | 30  | LEU  |
| 19  | XS    | 31  | ILE  |
| 19  | XS    | 37  | ARG  |
| 19  | XS    | 44  | MET  |
| 19  | XS    | 63  | THR  |
| 19  | XS    | 78  | ARG  |
| 19  | XS    | 81  | ARG  |
| 19  | XS    | 83  | HIS  |
| 20  | XT    | 10  | LEU  |
| 20  | XT    | 13  | LEU  |
| 20  | XT    | 24  | LEU  |
| 20  | XT    | 37  | SER  |
| 20  | XT    | 41  | ILE  |
| 20  | XT    | 45  | GLN  |
| 20  | XT    | 50  | GLU  |
| 20  | XT    | 73  | HIS  |
| 20  | XT    | 84  | LEU  |
| 20  | XT    | 93  | GLU  |
| 21  | XU    | 6   | ARG  |
| 27  | YD    | 5   | LYS  |
| 27  | YD    | 17  | THR  |
| 27  | YD    | 27  | THR  |
| 27  | YD    | 28  | GLU  |
| 27  | YD    | 30  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | YD    | 38  | LYS  |
| 27  | YD    | 43  | ARG  |
| 27  | YD    | 44  | ASN  |
| 27  | YD    | 49  | ILE  |
| 27  | YD    | 65  | ILE  |
| 27  | YD    | 73  | VAL  |
| 27  | YD    | 88  | ARG  |
| 27  | YD    | 94  | LEU  |
| 27  | YD    | 95  | LEU  |
| 27  | YD    | 103 | ARG  |
| 27  | YD    | 105 | ILE  |
| 27  | YD    | 106 | ILE  |
| 27  | YD    | 111 | LEU  |
| 27  | YD    | 112 | GLN  |
| 27  | YD    | 134 | ARG  |
| 27  | YD    | 141 | VAL  |
| 27  | YD    | 192 | THR  |
| 27  | YD    | 200 | ASP  |
| 27  | YD    | 202 | LYS  |
| 27  | YD    | 212 | SER  |
| 27  | YD    | 217 | ARG  |
| 27  | YD    | 218 | ARG  |
| 27  | YD    | 221 | VAL  |
| 27  | YD    | 229 | VAL  |
| 27  | YD    | 237 | GLU  |
| 27  | YD    | 242 | ARG  |
| 27  | YD    | 257 | LEU  |
| 27  | YD    | 259 | THR  |
| 27  | YD    | 273 | ARG  |
| 28  | YE    | 4   | ILE  |
| 28  | YE    | 12  | THR  |
| 28  | YE    | 13  | ARG  |
| 28  | YE    | 16  | ARG  |
| 28  | YE    | 17  | ASP  |
| 28  | YE    | 21  | VAL  |
| 28  | YE    | 23  | VAL  |
| 28  | YE    | 26  | ILE  |
| 28  | YE    | 27  | LEU  |
| 28  | YE    | 41  | LYS  |
| 28  | YE    | 42  | ASP  |
| 28  | YE    | 49  | LEU  |
| 28  | YE    | 77  | ILE  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 28         | YE           | 79         | ARG         |
| 28         | YE           | 82         | ARG         |
| 28         | YE           | 92         | THR         |
| 28         | YE           | 113        | PHE         |
| 28         | YE           | 116        | VAL         |
| 28         | YE           | 117        | MET         |
| 28         | YE           | 119        | ARG         |
| 28         | YE           | 127        | ASP         |
| 28         | YE           | 128        | SER         |
| 28         | YE           | 144        | ARG         |
| 28         | YE           | 146        | THR         |
| 28         | YE           | 154        | LYS         |
| 28         | YE           | 175        | VAL         |
| 28         | YE           | 197        | ILE         |
| 28         | YE           | 200        | GLU         |
| 28         | YE           | 202        | LYS         |
| 28         | YE           | 203        | LYS         |
| 29         | YF           | 9          | ILE         |
| 29         | YF           | 32         | LEU         |
| 29         | YF           | 33         | LEU         |
| 29         | YF           | 38         | ARG         |
| 29         | YF           | 45         | ARG         |
| 29         | YF           | 65         | TRP         |
| 29         | YF           | 70         | THR         |
| 29         | YF           | 78         | ILE         |
| 29         | YF           | 105        | VAL         |
| 29         | YF           | 106        | ARG         |
| 29         | YF           | 107        | LYS         |
| 29         | YF           | 117        | ARG         |
| 29         | YF           | 127        | GLU         |
| 29         | YF           | 161        | GLU         |
| 29         | YF           | 164        | ARG         |
| 29         | YF           | 165        | ARG         |
| 29         | YF           | 170        | LEU         |
| 29         | YF           | 174        | VAL         |
| 29         | YF           | 176        | LEU         |
| 29         | YF           | 181        | LEU         |
| 29         | YF           | 183        | VAL         |
| 29         | YF           | 196        | LEU         |
| 29         | YF           | 197        | ASP         |
| 29         | YF           | 206        | ILE         |
| 30         | YG           | 3          | LEU         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | YG    | 7   | LEU  |
| 30  | YG    | 22  | ARG  |
| 30  | YG    | 31  | VAL  |
| 30  | YG    | 34  | LEU  |
| 30  | YG    | 43  | LEU  |
| 30  | YG    | 45  | GLU  |
| 30  | YG    | 58  | GLN  |
| 30  | YG    | 63  | ILE  |
| 30  | YG    | 66  | GLN  |
| 30  | YG    | 67  | LYS  |
| 30  | YG    | 80  | PHE  |
| 30  | YG    | 82  | LEU  |
| 30  | YG    | 84  | LYS  |
| 30  | YG    | 88  | ILE  |
| 30  | YG    | 90  | LEU  |
| 30  | YG    | 94  | LEU  |
| 30  | YG    | 116 | ASP  |
| 30  | YG    | 118 | ARG  |
| 30  | YG    | 145 | THR  |
| 30  | YG    | 167 | GLU  |
| 31  | YH    | 3   | ARG  |
| 31  | YH    | 4   | ILE  |
| 31  | YH    | 6   | ARG  |
| 31  | YH    | 9   | ILE  |
| 31  | YH    | 13  | LYS  |
| 31  | YH    | 27  | LYS  |
| 31  | YH    | 32  | GLU  |
| 31  | YH    | 37  | VAL  |
| 31  | YH    | 40  | GLU  |
| 31  | YH    | 41  | MET  |
| 31  | YH    | 53  | GLU  |
| 31  | YH    | 59  | ARG  |
| 31  | YH    | 77  | LYS  |
| 31  | YH    | 88  | LEU  |
| 31  | YH    | 89  | ILE  |
| 31  | YH    | 103 | LEU  |
| 31  | YH    | 105 | LEU  |
| 31  | YH    | 122 | THR  |
| 31  | YH    | 129 | THR  |
| 31  | YH    | 132 | ARG  |
| 31  | YH    | 136 | ILE  |
| 31  | YH    | 143 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | YH    | 149 | ARG  |
| 31  | YH    | 152 | ARG  |
| 31  | YH    | 153 | LYS  |
| 31  | YH    | 169 | VAL  |
| 32  | YI    | 1   | MET  |
| 32  | YI    | 2   | LYS  |
| 32  | YI    | 9   | LEU  |
| 32  | YI    | 10  | GLU  |
| 32  | YI    | 20  | ASP  |
| 32  | YI    | 27  | ARG  |
| 32  | YI    | 33  | ARG  |
| 32  | YI    | 35  | LEU  |
| 32  | YI    | 38  | LEU  |
| 32  | YI    | 40  | THR  |
| 32  | YI    | 56  | LYS  |
| 32  | YI    | 67  | ARG  |
| 32  | YI    | 70  | GLU  |
| 32  | YI    | 85  | GLU  |
| 32  | YI    | 86  | THR  |
| 32  | YI    | 87  | LYS  |
| 32  | YI    | 88  | ILE  |
| 32  | YI    | 92  | VAL  |
| 32  | YI    | 101 | LEU  |
| 32  | YI    | 110 | ASP  |
| 32  | YI    | 112 | LYS  |
| 32  | YI    | 113 | ARG  |
| 32  | YI    | 130 | TYR  |
| 32  | YI    | 131 | LYS  |
| 32  | YI    | 135 | GLU  |
| 32  | YI    | 136 | VAL  |
| 32  | YI    | 138 | ILE  |
| 32  | YI    | 139 | GLN  |
| 32  | YI    | 140 | LEU  |
| 32  | YI    | 142 | VAL  |
| 33  | YN    | 2   | LYS  |
| 33  | YN    | 5   | VAL  |
| 33  | YN    | 7   | LYS  |
| 33  | YN    | 32  | THR  |
| 33  | YN    | 34  | LEU  |
| 33  | YN    | 43  | THR  |
| 33  | YN    | 48  | MET  |
| 33  | YN    | 60  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | YN    | 61  | ARG  |
| 33  | YN    | 62  | VAL  |
| 33  | YN    | 65  | LYS  |
| 33  | YN    | 67  | LEU  |
| 33  | YN    | 73  | THR  |
| 33  | YN    | 90  | MET  |
| 33  | YN    | 96  | GLU  |
| 33  | YN    | 99  | LEU  |
| 33  | YN    | 109 | LYS  |
| 33  | YN    | 112 | LEU  |
| 33  | YN    | 116 | LEU  |
| 33  | YN    | 120 | LEU  |
| 33  | YN    | 136 | GLU  |
| 34  | YO    | 9   | GLU  |
| 34  | YO    | 19  | ILE  |
| 34  | YO    | 20  | MET  |
| 34  | YO    | 23  | ARG  |
| 34  | YO    | 24  | VAL  |
| 34  | YO    | 31  | LYS  |
| 34  | YO    | 47  | ILE  |
| 34  | YO    | 49  | ARG  |
| 34  | YO    | 53  | LYS  |
| 34  | YO    | 66  | LYS  |
| 34  | YO    | 91  | LEU  |
| 35  | YP    | 6   | LEU  |
| 35  | YP    | 7   | ARG  |
| 35  | YP    | 10  | PRO  |
| 35  | YP    | 14  | LYS  |
| 35  | YP    | 16  | ARG  |
| 35  | YP    | 19  | VAL  |
| 35  | YP    | 21  | ARG  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 29  | LYS  |
| 35  | YP    | 32  | THR  |
| 35  | YP    | 36  | LYS  |
| 35  | YP    | 45  | LEU  |
| 35  | YP    | 49  | ARG  |
| 35  | YP    | 50  | ARG  |
| 35  | YP    | 61  | ARG  |
| 35  | YP    | 62  | LEU  |
| 35  | YP    | 64  | LYS  |
| 35  | YP    | 65  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | YP    | 71  | VAL  |
| 35  | YP    | 75  | ILE  |
| 35  | YP    | 88  | LEU  |
| 35  | YP    | 91  | PHE  |
| 35  | YP    | 94  | GLU  |
| 35  | YP    | 98  | GLU  |
| 35  | YP    | 100 | LEU  |
| 35  | YP    | 101 | VAL  |
| 35  | YP    | 112 | LEU  |
| 35  | YP    | 115 | LEU  |
| 35  | YP    | 117 | GLU  |
| 35  | YP    | 123 | LEU  |
| 35  | YP    | 135 | LEU  |
| 35  | YP    | 144 | GLU  |
| 35  | YP    | 146 | VAL  |
| 35  | YP    | 147 | LEU  |
| 35  | YP    | 149 | GLU  |
| 36  | YQ    | 5   | ARG  |
| 36  | YQ    | 10  | ARG  |
| 36  | YQ    | 25  | ASP  |
| 36  | YQ    | 45  | GLN  |
| 36  | YQ    | 55  | VAL  |
| 36  | YQ    | 59  | ARG  |
| 36  | YQ    | 71  | ASP  |
| 36  | YQ    | 75  | THR  |
| 36  | YQ    | 76  | LYS  |
| 36  | YQ    | 79  | LEU  |
| 36  | YQ    | 81  | VAL  |
| 36  | YQ    | 82  | ARG  |
| 36  | YQ    | 83  | MET  |
| 36  | YQ    | 87  | LYS  |
| 36  | YQ    | 103 | MET  |
| 36  | YQ    | 112 | GLU  |
| 36  | YQ    | 132 | VAL  |
| 36  | YQ    | 135 | ASP  |
| 36  | YQ    | 139 | GLU  |
| 37  | YR    | 1   | MET  |
| 37  | YR    | 18  | LEU  |
| 37  | YR    | 28  | LEU  |
| 37  | YR    | 29  | LEU  |
| 37  | YR    | 34  | ILE  |
| 37  | YR    | 36  | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 37         | YR           | 40         | LYS         |
| 37         | YR           | 44         | LEU         |
| 37         | YR           | 51         | LEU         |
| 37         | YR           | 54         | LEU         |
| 37         | YR           | 57         | ARG         |
| 37         | YR           | 63         | ARG         |
| 37         | YR           | 65         | LEU         |
| 37         | YR           | 79         | LEU         |
| 37         | YR           | 83         | ILE         |
| 37         | YR           | 91         | GLN         |
| 37         | YR           | 95         | THR         |
| 37         | YR           | 100        | LEU         |
| 37         | YR           | 102        | GLU         |
| 37         | YR           | 104        | ARG         |
| 37         | YR           | 105        | ARG         |
| 38         | YS           | 10         | ARG         |
| 38         | YS           | 12         | PHE         |
| 38         | YS           | 14         | VAL         |
| 38         | YS           | 15         | ARG         |
| 38         | YS           | 20         | ARG         |
| 38         | YS           | 25         | ARG         |
| 38         | YS           | 27         | SER         |
| 38         | YS           | 44         | LYS         |
| 38         | YS           | 54         | LEU         |
| 38         | YS           | 56         | LEU         |
| 38         | YS           | 58         | LEU         |
| 38         | YS           | 69         | VAL         |
| 38         | YS           | 78         | LEU         |
| 38         | YS           | 83         | LYS         |
| 38         | YS           | 85         | VAL         |
| 38         | YS           | 89         | ARG         |
| 38         | YS           | 103        | GLU         |
| 38         | YS           | 106        | ARG         |
| 38         | YS           | 111        | GLU         |
| 39         | YT           | 17         | THR         |
| 39         | YT           | 23         | ARG         |
| 39         | YT           | 27         | THR         |
| 39         | YT           | 28         | VAL         |
| 39         | YT           | 40         | THR         |
| 39         | YT           | 41         | ARG         |
| 39         | YT           | 42         | ILE         |
| 39         | YT           | 51         | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 39         | YT           | 58         | ASN         |
| 39         | YT           | 65         | LYS         |
| 39         | YT           | 66         | VAL         |
| 39         | YT           | 74         | ARG         |
| 39         | YT           | 86         | ILE         |
| 39         | YT           | 87         | ASP         |
| 39         | YT           | 88         | ILE         |
| 39         | YT           | 89         | VAL         |
| 39         | YT           | 110        | ILE         |
| 39         | YT           | 112        | ARG         |
| 39         | YT           | 115        | ARG         |
| 39         | YT           | 125        | ARG         |
| 39         | YT           | 128        | GLU         |
| 39         | YT           | 134        | GLU         |
| 40         | YU           | 5          | LYS         |
| 40         | YU           | 11         | ARG         |
| 40         | YU           | 27         | LEU         |
| 40         | YU           | 51         | LYS         |
| 40         | YU           | 52         | ARG         |
| 40         | YU           | 60         | LEU         |
| 40         | YU           | 64         | ARG         |
| 40         | YU           | 70         | ARG         |
| 40         | YU           | 74         | LEU         |
| 40         | YU           | 88         | ILE         |
| 40         | YU           | 91         | ASP         |
| 40         | YU           | 98         | LEU         |
| 40         | YU           | 104        | GLN         |
| 40         | YU           | 111        | GLU         |
| 40         | YU           | 112        | ARG         |
| 40         | YU           | 114        | LYS         |
| 41         | YV           | 7          | THR         |
| 41         | YV           | 10         | LYS         |
| 41         | YV           | 13         | ARG         |
| 41         | YV           | 19         | LYS         |
| 41         | YV           | 35         | LEU         |
| 41         | YV           | 39         | LEU         |
| 41         | YV           | 40         | LEU         |
| 41         | YV           | 45         | THR         |
| 41         | YV           | 61         | VAL         |
| 41         | YV           | 66         | ARG         |
| 41         | YV           | 72         | VAL         |
| 41         | YV           | 73         | SER         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | YV    | 78  | LYS  |
| 41  | YV    | 79  | VAL  |
| 41  | YV    | 99  | ILE  |
| 42  | YW    | 11  | ARG  |
| 42  | YW    | 16  | LYS  |
| 42  | YW    | 23  | LEU  |
| 42  | YW    | 37  | ARG  |
| 42  | YW    | 40  | ASN  |
| 42  | YW    | 51  | LEU  |
| 42  | YW    | 67  | ASP  |
| 42  | YW    | 69  | LEU  |
| 42  | YW    | 76  | VAL  |
| 42  | YW    | 88  | ARG  |
| 42  | YW    | 90  | ARG  |
| 42  | YW    | 92  | ARG  |
| 42  | YW    | 95  | ILE  |
| 42  | YW    | 96  | ILE  |
| 42  | YW    | 100 | THR  |
| 42  | YW    | 106 | ILE  |
| 42  | YW    | 107 | LEU  |
| 43  | YX    | 6   | ASP  |
| 43  | YX    | 12  | VAL  |
| 43  | YX    | 15  | GLU  |
| 43  | YX    | 27  | THR  |
| 43  | YX    | 36  | LYS  |
| 43  | YX    | 43  | VAL  |
| 43  | YX    | 49  | VAL  |
| 43  | YX    | 57  | LEU  |
| 43  | YX    | 59  | VAL  |
| 43  | YX    | 63  | LYS  |
| 43  | YX    | 65  | ARG  |
| 43  | YX    | 66  | LEU  |
| 43  | YX    | 80  | ILE  |
| 43  | YX    | 88  | LYS  |
| 44  | YY    | 14  | LEU  |
| 44  | YY    | 26  | LYS  |
| 44  | YY    | 27  | VAL  |
| 44  | YY    | 28  | LYS  |
| 44  | YY    | 29  | GLU  |
| 44  | YY    | 34  | LYS  |
| 44  | YY    | 38  | ILE  |
| 44  | YY    | 44  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | YY    | 57  | GLN  |
| 44  | YY    | 61  | ILE  |
| 44  | YY    | 64  | GLU  |
| 44  | YY    | 67  | LEU  |
| 44  | YY    | 71  | LYS  |
| 44  | YY    | 73  | ARG  |
| 44  | YY    | 75  | ILE  |
| 44  | YY    | 86  | ARG  |
| 44  | YY    | 87  | LYS  |
| 44  | YY    | 89  | PHE  |
| 44  | YY    | 90  | LEU  |
| 44  | YY    | 95  | LYS  |
| 44  | YY    | 97  | ARG  |
| 45  | YZ    | 2   | GLU  |
| 45  | YZ    | 5   | LEU  |
| 45  | YZ    | 8   | TYR  |
| 45  | YZ    | 10  | ARG  |
| 45  | YZ    | 18  | LEU  |
| 45  | YZ    | 19  | ARG  |
| 45  | YZ    | 20  | ARG  |
| 45  | YZ    | 31  | ARG  |
| 45  | YZ    | 41  | LEU  |
| 45  | YZ    | 53  | ILE  |
| 45  | YZ    | 74  | VAL  |
| 45  | YZ    | 76  | LEU  |
| 45  | YZ    | 81  | ARG  |
| 45  | YZ    | 93  | ASP  |
| 45  | YZ    | 112 | ARG  |
| 45  | YZ    | 122 | ARG  |
| 45  | YZ    | 129 | SER  |
| 45  | YZ    | 133 | ILE  |
| 45  | YZ    | 137 | ILE  |
| 45  | YZ    | 140 | ASP  |
| 45  | YZ    | 141 | VAL  |
| 45  | YZ    | 144 | LEU  |
| 45  | YZ    | 150 | LEU  |
| 45  | YZ    | 151 | HIS  |
| 45  | YZ    | 153 | SER  |
| 45  | YZ    | 156 | LYS  |
| 45  | YZ    | 163 | LEU  |
| 45  | YZ    | 166 | SER  |
| 45  | YZ    | 180 | VAL  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 46         | Y0           | 9          | SER         |
| 46         | Y0           | 11         | ARG         |
| 46         | Y0           | 36         | ILE         |
| 46         | Y0           | 55         | ARG         |
| 46         | Y0           | 64         | ASP         |
| 46         | Y0           | 74         | ARG         |
| 47         | Y1           | 30         | VAL         |
| 47         | Y1           | 46         | LEU         |
| 47         | Y1           | 50         | ARG         |
| 47         | Y1           | 51         | VAL         |
| 47         | Y1           | 56         | GLN         |
| 47         | Y1           | 62         | VAL         |
| 47         | Y1           | 78         | LYS         |
| 47         | Y1           | 80         | LEU         |
| 47         | Y1           | 82         | LEU         |
| 47         | Y1           | 83         | GLU         |
| 47         | Y1           | 91         | LYS         |
| 47         | Y1           | 92         | LYS         |
| 48         | Y2           | 4          | SER         |
| 48         | Y2           | 7          | ARG         |
| 48         | Y2           | 9          | GLN         |
| 48         | Y2           | 16         | LEU         |
| 48         | Y2           | 23         | LYS         |
| 48         | Y2           | 24         | LEU         |
| 48         | Y2           | 27         | GLU         |
| 48         | Y2           | 32         | LEU         |
| 48         | Y2           | 34         | GLU         |
| 48         | Y2           | 41         | ILE         |
| 48         | Y2           | 47         | ASN         |
| 48         | Y2           | 50         | ILE         |
| 48         | Y2           | 51         | ARG         |
| 48         | Y2           | 52         | ASP         |
| 48         | Y2           | 53         | LEU         |
| 48         | Y2           | 64         | LEU         |
| 48         | Y2           | 65         | ASN         |
| 49         | Y3           | 6          | VAL         |
| 49         | Y3           | 8          | LEU         |
| 49         | Y3           | 23         | LEU         |
| 49         | Y3           | 30         | ARG         |
| 49         | Y3           | 31         | LEU         |
| 49         | Y3           | 36         | VAL         |
| 49         | Y3           | 37         | LEU         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | Y3    | 56  | VAL  |
| 50  | Y4    | 6   | HIS  |
| 50  | Y4    | 10  | VAL  |
| 50  | Y4    | 15  | ILE  |
| 50  | Y4    | 16  | CYS  |
| 50  | Y4    | 22  | ILE  |
| 50  | Y4    | 27  | THR  |
| 50  | Y4    | 34  | GLU  |
| 50  | Y4    | 39  | CYS  |
| 50  | Y4    | 42  | PHE  |
| 50  | Y4    | 43  | TYR  |
| 50  | Y4    | 48  | ARG  |
| 50  | Y4    | 49  | PHE  |
| 50  | Y4    | 53  | GLU  |
| 50  | Y4    | 57  | GLU  |
| 50  | Y4    | 58  | ARG  |
| 50  | Y4    | 61  | ARG  |
| 50  | Y4    | 63  | TYR  |
| 50  | Y4    | 67  | TYR  |
| 50  | Y4    | 68  | ARG  |
| 50  | Y4    | 71  | ARG  |
| 51  | Y5    | 3   | LYS  |
| 51  | Y5    | 4   | HIS  |
| 51  | Y5    | 6   | VAL  |
| 51  | Y5    | 11  | THR  |
| 51  | Y5    | 29  | THR  |
| 51  | Y5    | 36  | CYS  |
| 51  | Y5    | 37  | LYS  |
| 51  | Y5    | 40  | LYS  |
| 51  | Y5    | 48  | GLU  |
| 51  | Y5    | 51  | TYR  |
| 51  | Y5    | 52  | TYR  |
| 51  | Y5    | 56  | LYS  |
| 51  | Y5    | 58  | LEU  |
| 52  | Y6    | 6   | ARG  |
| 52  | Y6    | 8   | LYS  |
| 52  | Y6    | 11  | LEU  |
| 52  | Y6    | 19  | ARG  |
| 52  | Y6    | 23  | THR  |
| 52  | Y6    | 30  | THR  |
| 52  | Y6    | 33  | LYS  |
| 52  | Y6    | 34  | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 52         | Y6           | 37         | ARG         |
| 52         | Y6           | 44         | ARG         |
| 53         | Y7           | 1          | MET         |
| 53         | Y7           | 4          | THR         |
| 53         | Y7           | 8          | ASN         |
| 53         | Y7           | 9          | ARG         |
| 53         | Y7           | 10         | ARG         |
| 53         | Y7           | 14         | LYS         |
| 53         | Y7           | 47         | ARG         |
| 54         | Y8           | 13         | ARG         |
| 54         | Y8           | 14         | VAL         |
| 54         | Y8           | 15         | LYS         |
| 54         | Y8           | 29         | LYS         |
| 54         | Y8           | 30         | ARG         |
| 54         | Y8           | 34         | TRP         |
| 54         | Y8           | 43         | GLN         |
| 54         | Y8           | 44         | LYS         |
| 54         | Y8           | 47         | LYS         |
| 54         | Y8           | 56         | GLU         |
| 54         | Y8           | 58         | ILE         |
| 54         | Y8           | 64         | TYR         |
| 54         | Y8           | 65         | GLU         |
| 55         | Y9           | 1          | MET         |
| 55         | Y9           | 17         | ILE         |
| 56         | Z8           | 7          | LYS         |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | QB           | 19         | HIS         |
| 2          | QB           | 204        | ASN         |
| 2          | QB           | 212        | GLN         |
| 10         | QJ           | 13         | HIS         |
| 10         | QJ           | 78         | ASN         |
| 13         | QM           | 77         | ASN         |
| 13         | QM           | 92         | HIS         |
| 19         | QS           | 47         | HIS         |
| 38         | RS           | 34         | HIS         |
| 43         | RX           | 55         | ASN         |
| 51         | R5           | 22         | HIS         |
| 55         | R9           | 29         | ASN         |
| 55         | R9           | 32         | HIS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | XB    | 19  | HIS  |
| 2   | XB    | 204 | ASN  |
| 2   | XB    | 212 | GLN  |
| 10  | XJ    | 78  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1499/1522 (98%) | 267 (17%)         | 43 (2%)         |
| 1   | XA    | 1498/1522 (98%) | 277 (18%)         | 38 (2%)         |
| 22  | QV    | 76/77 (98%)     | 19 (25%)          | 1 (1%)          |
| 22  | XV    | 76/77 (98%)     | 17 (22%)          | 1 (1%)          |
| 23  | QW    | 75/76 (98%)     | 16 (21%)          | 0               |
| 23  | QY    | 15/76 (19%)     | 3 (20%)           | 0               |
| 23  | XW    | 75/76 (98%)     | 19 (25%)          | 0               |
| 23  | XY    | 15/76 (19%)     | 4 (26%)           | 0               |
| 24  | QX    | 9/24 (37%)      | 0                 | 0               |
| 24  | XX    | 9/24 (37%)      | 0                 | 0               |
| 25  | RA    | 2879/2915 (98%) | 567 (19%)         | 57 (1%)         |
| 25  | YA    | 2880/2915 (98%) | 563 (19%)         | 57 (1%)         |
| 26  | RB    | 119/122 (97%)   | 21 (17%)          | 1 (0%)          |
| 26  | YB    | 119/122 (97%)   | 21 (17%)          | 1 (0%)          |
| All | All   | 9344/9624 (97%) | 1794 (19%)        | 199 (2%)        |

All (1794) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 6   | G    |
| 1   | QA    | 7   | G    |
| 1   | QA    | 22  | G    |
| 1   | QA    | 32  | A    |
| 1   | QA    | 39  | G    |
| 1   | QA    | 47  | C    |
| 1   | QA    | 48  | C    |
| 1   | QA    | 51  | A    |
| 1   | QA    | 64  | G    |
| 1   | QA    | 65  | U    |
| 1   | QA    | 66  | G    |
| 1   | QA    | 76  | G    |
| 1   | QA    | 79  | G    |
| 1   | QA    | 80  | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 90     | C    |
| 1   | QA    | 91     | C    |
| 1   | QA    | 95     | G    |
| 1   | QA    | 101    | A    |
| 1   | QA    | 116    | A    |
| 1   | QA    | 120    | A    |
| 1   | QA    | 121    | C    |
| 1   | QA    | 129(A) | G    |
| 1   | QA    | 144    | G    |
| 1   | QA    | 146    | G    |
| 1   | QA    | 147    | G    |
| 1   | QA    | 163    | C    |
| 1   | QA    | 169    | C    |
| 1   | QA    | 171    | A    |
| 1   | QA    | 173    | U    |
| 1   | QA    | 174    | C    |
| 1   | QA    | 182    | U    |
| 1   | QA    | 190    | G    |
| 1   | QA    | 191(A) | G    |
| 1   | QA    | 195    | A    |
| 1   | QA    | 197    | A    |
| 1   | QA    | 209    | U    |
| 1   | QA    | 210    | U    |
| 1   | QA    | 216    | G    |
| 1   | QA    | 244    | U    |
| 1   | QA    | 245    | C    |
| 1   | QA    | 247    | G    |
| 1   | QA    | 251    | G    |
| 1   | QA    | 267    | C    |
| 1   | QA    | 270    | A    |
| 1   | QA    | 281    | G    |
| 1   | QA    | 289    | G    |
| 1   | QA    | 321    | A    |
| 1   | QA    | 328    | C    |
| 1   | QA    | 329    | A    |
| 1   | QA    | 332    | G    |
| 1   | QA    | 344    | A    |
| 1   | QA    | 346    | G    |
| 1   | QA    | 347    | G    |
| 1   | QA    | 351    | G    |
| 1   | QA    | 352    | C    |
| 1   | QA    | 353    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 354 | G    |
| 1   | QA    | 356 | A    |
| 1   | QA    | 367 | U    |
| 1   | QA    | 372 | C    |
| 1   | QA    | 373 | A    |
| 1   | QA    | 390 | C    |
| 1   | QA    | 397 | A    |
| 1   | QA    | 398 | C    |
| 1   | QA    | 406 | G    |
| 1   | QA    | 411 | A    |
| 1   | QA    | 412 | A    |
| 1   | QA    | 413 | G    |
| 1   | QA    | 414 | A    |
| 1   | QA    | 421 | U    |
| 1   | QA    | 422 | C    |
| 1   | QA    | 423 | G    |
| 1   | QA    | 424 | G    |
| 1   | QA    | 429 | U    |
| 1   | QA    | 430 | A    |
| 1   | QA    | 442 | C    |
| 1   | QA    | 452 | A    |
| 1   | QA    | 465 | A    |
| 1   | QA    | 466 | C    |
| 1   | QA    | 482 | A    |
| 1   | QA    | 485 | G    |
| 1   | QA    | 486 | U    |
| 1   | QA    | 496 | A    |
| 1   | QA    | 497 | U    |
| 1   | QA    | 505 | G    |
| 1   | QA    | 509 | A    |
| 1   | QA    | 510 | A    |
| 1   | QA    | 511 | C    |
| 1   | QA    | 518 | C    |
| 1   | QA    | 527 | G    |
| 1   | QA    | 531 | U    |
| 1   | QA    | 532 | A    |
| 1   | QA    | 533 | A    |
| 1   | QA    | 534 | U    |
| 1   | QA    | 545 | C    |
| 1   | QA    | 547 | A    |
| 1   | QA    | 559 | A    |
| 1   | QA    | 561 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 562 | C    |
| 1   | QA    | 564 | C    |
| 1   | QA    | 566 | G    |
| 1   | QA    | 568 | G    |
| 1   | QA    | 572 | A    |
| 1   | QA    | 573 | A    |
| 1   | QA    | 576 | G    |
| 1   | QA    | 577 | G    |
| 1   | QA    | 596 | C    |
| 1   | QA    | 618 | C    |
| 1   | QA    | 630 | G    |
| 1   | QA    | 631 | G    |
| 1   | QA    | 632 | A    |
| 1   | QA    | 653 | A    |
| 1   | QA    | 665 | A    |
| 1   | QA    | 666 | G    |
| 1   | QA    | 688 | G    |
| 1   | QA    | 701 | C    |
| 1   | QA    | 702 | A    |
| 1   | QA    | 703 | G    |
| 1   | QA    | 704 | A    |
| 1   | QA    | 723 | U    |
| 1   | QA    | 731 | G    |
| 1   | QA    | 748 | C    |
| 1   | QA    | 754 | C    |
| 1   | QA    | 755 | G    |
| 1   | QA    | 777 | A    |
| 1   | QA    | 786 | G    |
| 1   | QA    | 792 | A    |
| 1   | QA    | 793 | U    |
| 1   | QA    | 794 | A    |
| 1   | QA    | 813 | U    |
| 1   | QA    | 817 | C    |
| 1   | QA    | 819 | A    |
| 1   | QA    | 821 | G    |
| 1   | QA    | 828 | A    |
| 1   | QA    | 841 | U    |
| 1   | QA    | 843 | U    |
| 1   | QA    | 848 | C    |
| 1   | QA    | 859 | A    |
| 1   | QA    | 871 | U    |
| 1   | QA    | 872 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 902     | G    |
| 1   | QA    | 914     | A    |
| 1   | QA    | 927     | G    |
| 1   | QA    | 934     | C    |
| 1   | QA    | 935     | A    |
| 1   | QA    | 960     | U    |
| 1   | QA    | 961     | U    |
| 1   | QA    | 968     | A    |
| 1   | QA    | 969     | A    |
| 1   | QA    | 971     | G    |
| 1   | QA    | 974     | A    |
| 1   | QA    | 975     | A    |
| 1   | QA    | 976     | G    |
| 1   | QA    | 977     | A    |
| 1   | QA    | 980     | C    |
| 1   | QA    | 983     | A    |
| 1   | QA    | 991     | U    |
| 1   | QA    | 992     | U    |
| 1   | QA    | 993     | G    |
| 1   | QA    | 994     | A    |
| 1   | QA    | 1001    | G    |
| 1   | QA    | 1004    | A    |
| 1   | QA    | 1006    | C    |
| 1   | QA    | 1009    | G    |
| 1   | QA    | 1021    | G    |
| 1   | QA    | 1024    | G    |
| 1   | QA    | 1025    | U    |
| 1   | QA    | 1028    | C    |
| 1   | QA    | 1029    | G    |
| 1   | QA    | 1032(A) | G    |
| 1   | QA    | 1036    | G    |
| 1   | QA    | 1040    | U    |
| 1   | QA    | 1046    | A    |
| 1   | QA    | 1053    | G    |
| 1   | QA    | 1054    | C    |
| 1   | QA    | 1055    | A    |
| 1   | QA    | 1064    | G    |
| 1   | QA    | 1065    | U    |
| 1   | QA    | 1066    | C    |
| 1   | QA    | 1081    | G    |
| 1   | QA    | 1094    | G    |
| 1   | QA    | 1095    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | QA    | 1101 | A    |
| 1   | QA    | 1124 | G    |
| 1   | QA    | 1125 | U    |
| 1   | QA    | 1126 | U    |
| 1   | QA    | 1130 | A    |
| 1   | QA    | 1131 | G    |
| 1   | QA    | 1136 | U    |
| 1   | QA    | 1137 | C    |
| 1   | QA    | 1138 | G    |
| 1   | QA    | 1139 | G    |
| 1   | QA    | 1145 | C    |
| 1   | QA    | 1146 | A    |
| 1   | QA    | 1157 | A    |
| 1   | QA    | 1158 | C    |
| 1   | QA    | 1159 | U    |
| 1   | QA    | 1160 | G    |
| 1   | QA    | 1163 | C    |
| 1   | QA    | 1178 | G    |
| 1   | QA    | 1181 | G    |
| 1   | QA    | 1182 | G    |
| 1   | QA    | 1183 | A    |
| 1   | QA    | 1187 | G    |
| 1   | QA    | 1196 | U    |
| 1   | QA    | 1197 | G    |
| 1   | QA    | 1200 | C    |
| 1   | QA    | 1201 | A    |
| 1   | QA    | 1202 | G    |
| 1   | QA    | 1212 | U    |
| 1   | QA    | 1213 | A    |
| 1   | QA    | 1215 | G    |
| 1   | QA    | 1226 | C    |
| 1   | QA    | 1238 | A    |
| 1   | QA    | 1241 | G    |
| 1   | QA    | 1256 | A    |
| 1   | QA    | 1257 | U    |
| 1   | QA    | 1258 | G    |
| 1   | QA    | 1260 | C    |
| 1   | QA    | 1270 | C    |
| 1   | QA    | 1280 | A    |
| 1   | QA    | 1281 | U    |
| 1   | QA    | 1282 | C    |
| 1   | QA    | 1286 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 1287    | A    |
| 1   | QA    | 1297    | C    |
| 1   | QA    | 1298    | C    |
| 1   | QA    | 1299    | A    |
| 1   | QA    | 1300    | G    |
| 1   | QA    | 1301    | U    |
| 1   | QA    | 1302    | U    |
| 1   | QA    | 1305    | G    |
| 1   | QA    | 1319    | A    |
| 1   | QA    | 1320    | C    |
| 1   | QA    | 1321    | C    |
| 1   | QA    | 1322    | C    |
| 1   | QA    | 1323    | G    |
| 1   | QA    | 1331    | G    |
| 1   | QA    | 1335    | C    |
| 1   | QA    | 1336    | C    |
| 1   | QA    | 1337    | G    |
| 1   | QA    | 1346    | A    |
| 1   | QA    | 1347    | G    |
| 1   | QA    | 1348    | U    |
| 1   | QA    | 1353    | G    |
| 1   | QA    | 1362(A) | C    |
| 1   | QA    | 1397    | C    |
| 1   | QA    | 1398    | A    |
| 1   | QA    | 1406    | U    |
| 1   | QA    | 1419    | G    |
| 1   | QA    | 1442    | G    |
| 1   | QA    | 1446    | A    |
| 1   | QA    | 1447    | G    |
| 1   | QA    | 1452    | C    |
| 1   | QA    | 1453    | G    |
| 1   | QA    | 1454    | G    |
| 1   | QA    | 1487    | G    |
| 1   | QA    | 1492    | A    |
| 1   | QA    | 1499    | A    |
| 1   | QA    | 1504    | G    |
| 1   | QA    | 1505    | G    |
| 1   | QA    | 1506    | U    |
| 1   | QA    | 1517    | G    |
| 1   | QA    | 1519    | A    |
| 1   | QA    | 1520    | G    |
| 1   | QA    | 1529    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | QA    | 1530 | G    |
| 22  | QV    | 3    | G    |
| 22  | QV    | 4    | G    |
| 22  | QV    | 7    | U    |
| 22  | QV    | 15   | C    |
| 22  | QV    | 17   | U    |
| 22  | QV    | 18   | G    |
| 22  | QV    | 19   | G    |
| 22  | QV    | 21   | A    |
| 22  | QV    | 22   | G    |
| 22  | QV    | 31   | G    |
| 22  | QV    | 47   | U    |
| 22  | QV    | 48   | C    |
| 22  | QV    | 52   | G    |
| 22  | QV    | 53   | G    |
| 22  | QV    | 54   | U    |
| 22  | QV    | 64   | G    |
| 22  | QV    | 67   | C    |
| 22  | QV    | 75   | C    |
| 22  | QV    | 76   | A    |
| 23  | QW    | 6    | G    |
| 23  | QW    | 14   | A    |
| 23  | QW    | 16   | U    |
| 23  | QW    | 17   | C    |
| 23  | QW    | 18   | G    |
| 23  | QW    | 19   | G    |
| 23  | QW    | 21   | A    |
| 23  | QW    | 37   | A    |
| 23  | QW    | 41   | C    |
| 23  | QW    | 43   | C    |
| 23  | QW    | 45   | U    |
| 23  | QW    | 47   | U    |
| 23  | QW    | 48   | C    |
| 23  | QW    | 57   | G    |
| 23  | QW    | 59   | U    |
| 23  | QW    | 71   | G    |
| 23  | QY    | 29   | G    |
| 23  | QY    | 36   | A    |
| 23  | QY    | 37   | A    |
| 25  | RA    | 9    | U    |
| 25  | RA    | 15   | G    |
| 25  | RA    | 28   | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 34         | C           |
| 25         | RA           | 35         | G           |
| 25         | RA           | 46         | C           |
| 25         | RA           | 51         | G           |
| 25         | RA           | 55         | G           |
| 25         | RA           | 72         | U           |
| 25         | RA           | 74         | A           |
| 25         | RA           | 75         | G           |
| 25         | RA           | 96         | G           |
| 25         | RA           | 101        | G           |
| 25         | RA           | 102        | G           |
| 25         | RA           | 103        | A           |
| 25         | RA           | 118        | A           |
| 25         | RA           | 120        | U           |
| 25         | RA           | 131        | G           |
| 25         | RA           | 138        | G           |
| 25         | RA           | 161        | U           |
| 25         | RA           | 177        | G           |
| 25         | RA           | 181        | A           |
| 25         | RA           | 196        | A           |
| 25         | RA           | 199        | A           |
| 25         | RA           | 206        | U           |
| 25         | RA           | 214        | G           |
| 25         | RA           | 215        | G           |
| 25         | RA           | 216        | A           |
| 25         | RA           | 221        | A           |
| 25         | RA           | 222        | A           |
| 25         | RA           | 223        | A           |
| 25         | RA           | 224        | G           |
| 25         | RA           | 226        | G           |
| 25         | RA           | 228        | A           |
| 25         | RA           | 229        | A           |
| 25         | RA           | 230        | U           |
| 25         | RA           | 232        | G           |
| 25         | RA           | 233        | A           |
| 25         | RA           | 242        | G           |
| 25         | RA           | 243        | U           |
| 25         | RA           | 248        | G           |
| 25         | RA           | 249        | C           |
| 25         | RA           | 250        | G           |
| 25         | RA           | 252        | G           |
| 25         | RA           | 265        | A           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 266    | G    |
| 25  | RA    | 269    | U    |
| 25  | RA    | 270(L) | U    |
| 25  | RA    | 270(M) | U    |
| 25  | RA    | 270(N) | G    |
| 25  | RA    | 270(P) | C    |
| 25  | RA    | 271(A) | C    |
| 25  | RA    | 271(B) | G    |
| 25  | RA    | 271(C) | U    |
| 25  | RA    | 271    | G    |
| 25  | RA    | 275    | G    |
| 25  | RA    | 276    | A    |
| 25  | RA    | 277    | C    |
| 25  | RA    | 278    | A    |
| 25  | RA    | 279    | C    |
| 25  | RA    | 299    | A    |
| 25  | RA    | 300    | A    |
| 25  | RA    | 311    | A    |
| 25  | RA    | 317    | G    |
| 25  | RA    | 323    | G    |
| 25  | RA    | 324    | A    |
| 25  | RA    | 329    | G    |
| 25  | RA    | 330    | A    |
| 25  | RA    | 342    | G    |
| 25  | RA    | 346    | A    |
| 25  | RA    | 352    | G    |
| 25  | RA    | 364    | C    |
| 25  | RA    | 371    | A    |
| 25  | RA    | 372    | G    |
| 25  | RA    | 373    | U    |
| 25  | RA    | 386    | G    |
| 25  | RA    | 404    | C    |
| 25  | RA    | 405    | U    |
| 25  | RA    | 411    | G    |
| 25  | RA    | 412    | A    |
| 25  | RA    | 428    | A    |
| 25  | RA    | 444    | C    |
| 25  | RA    | 448    | U    |
| 25  | RA    | 454    | A    |
| 25  | RA    | 457    | A    |
| 25  | RA    | 470    | A    |
| 25  | RA    | 481    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 504    | U    |
| 25  | RA    | 505    | A    |
| 25  | RA    | 509    | C    |
| 25  | RA    | 513    | A    |
| 25  | RA    | 527    | C    |
| 25  | RA    | 529    | A    |
| 25  | RA    | 531    | C    |
| 25  | RA    | 532    | A    |
| 25  | RA    | 533    | G    |
| 25  | RA    | 537    | C    |
| 25  | RA    | 539    | G    |
| 25  | RA    | 540    | G    |
| 25  | RA    | 546    | C    |
| 25  | RA    | 547    | A    |
| 25  | RA    | 556    | G    |
| 25  | RA    | 563    | G    |
| 25  | RA    | 568    | U    |
| 25  | RA    | 573    | G    |
| 25  | RA    | 574    | C    |
| 25  | RA    | 575    | A    |
| 25  | RA    | 588    | U    |
| 25  | RA    | 603    | A    |
| 25  | RA    | 607    | U    |
| 25  | RA    | 614    | U    |
| 25  | RA    | 615    | G    |
| 25  | RA    | 617    | G    |
| 25  | RA    | 621    | A    |
| 25  | RA    | 626    | U    |
| 25  | RA    | 627    | A    |
| 25  | RA    | 637    | A    |
| 25  | RA    | 638    | G    |
| 25  | RA    | 645    | C    |
| 25  | RA    | 646    | A    |
| 25  | RA    | 651    | G    |
| 25  | RA    | 652    | C    |
| 25  | RA    | 654    | A    |
| 25  | RA    | 654(A) | G    |
| 25  | RA    | 668    | G    |
| 25  | RA    | 669    | G    |
| 25  | RA    | 670    | A    |
| 25  | RA    | 686    | G    |
| 25  | RA    | 702    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | RA    | 717 | G    |
| 25  | RA    | 721 | C    |
| 25  | RA    | 722 | A    |
| 25  | RA    | 730 | C    |
| 25  | RA    | 776 | G    |
| 25  | RA    | 782 | A    |
| 25  | RA    | 784 | A    |
| 25  | RA    | 785 | G    |
| 25  | RA    | 789 | A    |
| 25  | RA    | 790 | C    |
| 25  | RA    | 805 | G    |
| 25  | RA    | 812 | C    |
| 25  | RA    | 819 | A    |
| 25  | RA    | 827 | U    |
| 25  | RA    | 828 | U    |
| 25  | RA    | 846 | C    |
| 25  | RA    | 847 | U    |
| 25  | RA    | 856 | C    |
| 25  | RA    | 857 | C    |
| 25  | RA    | 859 | G    |
| 25  | RA    | 860 | U    |
| 25  | RA    | 869 | G    |
| 25  | RA    | 872 | A    |
| 25  | RA    | 881 | G    |
| 25  | RA    | 884 | C    |
| 25  | RA    | 885 | C    |
| 25  | RA    | 886 | C    |
| 25  | RA    | 888 | C    |
| 25  | RA    | 889 | C    |
| 25  | RA    | 893 | C    |
| 25  | RA    | 896 | A    |
| 25  | RA    | 897 | C    |
| 25  | RA    | 899 | A    |
| 25  | RA    | 900 | A    |
| 25  | RA    | 901 | A    |
| 25  | RA    | 904 | C    |
| 25  | RA    | 907 | U    |
| 25  | RA    | 910 | A    |
| 25  | RA    | 917 | A    |
| 25  | RA    | 932 | G    |
| 25  | RA    | 941 | A    |
| 25  | RA    | 945 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 946    | G    |
| 25  | RA    | 961    | C    |
| 25  | RA    | 974    | G    |
| 25  | RA    | 974(A) | C    |
| 25  | RA    | 975    | G    |
| 25  | RA    | 980    | A    |
| 25  | RA    | 983    | A    |
| 25  | RA    | 996    | A    |
| 25  | RA    | 1003   | G    |
| 25  | RA    | 1011   | G    |
| 25  | RA    | 1012   | U    |
| 25  | RA    | 1013   | C    |
| 25  | RA    | 1015   | G    |
| 25  | RA    | 1017   | G    |
| 25  | RA    | 1020   | A    |
| 25  | RA    | 1023   | U    |
| 25  | RA    | 1025   | G    |
| 25  | RA    | 1026   | U    |
| 25  | RA    | 1027   | A    |
| 25  | RA    | 1033   | U    |
| 25  | RA    | 1044   | G    |
| 25  | RA    | 1045   | A    |
| 25  | RA    | 1046   | A    |
| 25  | RA    | 1050   | A    |
| 25  | RA    | 1054   | A    |
| 25  | RA    | 1055   | G    |
| 25  | RA    | 1057   | A    |
| 25  | RA    | 1059   | G    |
| 25  | RA    | 1060   | U    |
| 25  | RA    | 1061   | U    |
| 25  | RA    | 1065   | U    |
| 25  | RA    | 1066   | U    |
| 25  | RA    | 1067   | A    |
| 25  | RA    | 1068   | G    |
| 25  | RA    | 1069   | A    |
| 25  | RA    | 1070   | A    |
| 25  | RA    | 1071   | G    |
| 25  | RA    | 1076   | C    |
| 25  | RA    | 1077   | A    |
| 25  | RA    | 1078   | U    |
| 25  | RA    | 1079   | C    |
| 25  | RA    | 1080   | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1082       | U           |
| 25         | RA           | 1083       | U           |
| 25         | RA           | 1084       | A           |
| 25         | RA           | 1085       | A           |
| 25         | RA           | 1086       | A           |
| 25         | RA           | 1087       | G           |
| 25         | RA           | 1088       | A           |
| 25         | RA           | 1091       | G           |
| 25         | RA           | 1093       | G           |
| 25         | RA           | 1095       | A           |
| 25         | RA           | 1096       | A           |
| 25         | RA           | 1104       | C           |
| 25         | RA           | 1110       | G           |
| 25         | RA           | 1111       | A           |
| 25         | RA           | 1112       | G           |
| 25         | RA           | 1122       | G           |
| 25         | RA           | 1130       | U           |
| 25         | RA           | 1131       | G           |
| 25         | RA           | 1135       | C           |
| 25         | RA           | 1136       | G           |
| 25         | RA           | 1142       | U           |
| 25         | RA           | 1142(A)    | A           |
| 25         | RA           | 1151       | G           |
| 25         | RA           | 1155       | A           |
| 25         | RA           | 1170       | G           |
| 25         | RA           | 1173       | G           |
| 25         | RA           | 1174       | A           |
| 25         | RA           | 1175       | U           |
| 25         | RA           | 1176       | G           |
| 25         | RA           | 1178       | C           |
| 25         | RA           | 1179       | C           |
| 25         | RA           | 1180       | C           |
| 25         | RA           | 1183       | G           |
| 25         | RA           | 1195       | G           |
| 25         | RA           | 1204       | A           |
| 25         | RA           | 1205       | U           |
| 25         | RA           | 1206       | G           |
| 25         | RA           | 1210       | A           |
| 25         | RA           | 1211       | U           |
| 25         | RA           | 1220       | A           |
| 25         | RA           | 1221       | C           |
| 25         | RA           | 1236       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 1238    | G    |
| 25  | RA    | 1252    | G    |
| 25  | RA    | 1253    | A    |
| 25  | RA    | 1256    | G    |
| 25  | RA    | 1265    | A    |
| 25  | RA    | 1271    | G    |
| 25  | RA    | 1272    | A    |
| 25  | RA    | 1273    | U    |
| 25  | RA    | 1288    | U    |
| 25  | RA    | 1300    | U    |
| 25  | RA    | 1301    | A    |
| 25  | RA    | 1312    | U    |
| 25  | RA    | 1313    | U    |
| 25  | RA    | 1314    | C    |
| 25  | RA    | 1321    | A    |
| 25  | RA    | 1329    | U    |
| 25  | RA    | 1332    | G    |
| 25  | RA    | 1349    | A    |
| 25  | RA    | 1365    | A    |
| 25  | RA    | 1368    | G    |
| 25  | RA    | 1370    | C    |
| 25  | RA    | 1379    | A    |
| 25  | RA    | 1380    | G    |
| 25  | RA    | 1384    | A    |
| 25  | RA    | 1385    | G    |
| 25  | RA    | 1386    | C    |
| 25  | RA    | 1407    | C    |
| 25  | RA    | 1408    | C    |
| 25  | RA    | 1411    | C    |
| 25  | RA    | 1412    | A    |
| 25  | RA    | 1416    | G    |
| 25  | RA    | 1419    | A    |
| 25  | RA    | 1420    | U    |
| 25  | RA    | 1421    | G    |
| 25  | RA    | 1428    | C    |
| 25  | RA    | 1444(A) | A    |
| 25  | RA    | 1445    | C    |
| 25  | RA    | 1449    | A    |
| 25  | RA    | 1449(A) | G    |
| 25  | RA    | 1455    | G    |
| 25  | RA    | 1458    | C    |
| 25  | RA    | 1460    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1461       | G           |
| 25         | RA           | 1467       | C           |
| 25         | RA           | 1471       | A           |
| 25         | RA           | 1482       | U           |
| 25         | RA           | 1483       | G           |
| 25         | RA           | 1485       | G           |
| 25         | RA           | 1493       | C           |
| 25         | RA           | 1497       | U           |
| 25         | RA           | 1505       | C           |
| 25         | RA           | 1506       | C           |
| 25         | RA           | 1507       | A           |
| 25         | RA           | 1508       | A           |
| 25         | RA           | 1510       | A           |
| 25         | RA           | 1514       | U           |
| 25         | RA           | 1519       | G           |
| 25         | RA           | 1522       | G           |
| 25         | RA           | 1534       | G           |
| 25         | RA           | 1535       | U           |
| 25         | RA           | 1536       | A           |
| 25         | RA           | 1537       | C           |
| 25         | RA           | 1538       | G           |
| 25         | RA           | 1543       | A           |
| 25         | RA           | 1544       | C           |
| 25         | RA           | 1545       | A           |
| 25         | RA           | 1547       | C           |
| 25         | RA           | 1558       | A           |
| 25         | RA           | 1559       | G           |
| 25         | RA           | 1569       | A           |
| 25         | RA           | 1578       | U           |
| 25         | RA           | 1579       | A           |
| 25         | RA           | 1580       | A           |
| 25         | RA           | 1581       | G           |
| 25         | RA           | 1585       | C           |
| 25         | RA           | 1586       | A           |
| 25         | RA           | 1598       | C           |
| 25         | RA           | 1608       | A           |
| 25         | RA           | 1609       | A           |
| 25         | RA           | 1610       | A           |
| 25         | RA           | 1616       | A           |
| 25         | RA           | 1617       | C           |
| 25         | RA           | 1618       | A           |
| 25         | RA           | 1640       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1646       | C           |
| 25         | RA           | 1648       | C           |
| 25         | RA           | 1654       | A           |
| 25         | RA           | 1667       | G           |
| 25         | RA           | 1674       | G           |
| 25         | RA           | 1675       | C           |
| 25         | RA           | 1688       | U           |
| 25         | RA           | 1695       | G           |
| 25         | RA           | 1725       | G           |
| 25         | RA           | 1729       | A           |
| 25         | RA           | 1730       | U           |
| 25         | RA           | 1731       | G           |
| 25         | RA           | 1732       | A           |
| 25         | RA           | 1733       | G           |
| 25         | RA           | 1742       | C           |
| 25         | RA           | 1743       | G           |
| 25         | RA           | 1756       | G           |
| 25         | RA           | 1763       | G           |
| 25         | RA           | 1764       | G           |
| 25         | RA           | 1773       | A           |
| 25         | RA           | 1780       | A           |
| 25         | RA           | 1782       | C           |
| 25         | RA           | 1791       | A           |
| 25         | RA           | 1799       | G           |
| 25         | RA           | 1800       | C           |
| 25         | RA           | 1801       | G           |
| 25         | RA           | 1816       | G           |
| 25         | RA           | 1820       | U           |
| 25         | RA           | 1829       | A           |
| 25         | RA           | 1835       | G           |
| 25         | RA           | 1847       | A           |
| 25         | RA           | 1848       | A           |
| 25         | RA           | 1858       | G           |
| 25         | RA           | 1869       | G           |
| 25         | RA           | 1870       | C           |
| 25         | RA           | 1872       | A           |
| 25         | RA           | 1878       | G           |
| 25         | RA           | 1882       | C           |
| 25         | RA           | 1888       | G           |
| 25         | RA           | 1889       | A           |
| 25         | RA           | 1906       | G           |
| 25         | RA           | 1913       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1929       | G           |
| 25         | RA           | 1930       | G           |
| 25         | RA           | 1931       | U           |
| 25         | RA           | 1937       | A           |
| 25         | RA           | 1938       | A           |
| 25         | RA           | 1939       | U           |
| 25         | RA           | 1955       | U           |
| 25         | RA           | 1963       | U           |
| 25         | RA           | 1964       | G           |
| 25         | RA           | 1967       | C           |
| 25         | RA           | 1969       | A           |
| 25         | RA           | 1970       | A           |
| 25         | RA           | 1971       | A           |
| 25         | RA           | 1972       | A           |
| 25         | RA           | 1981       | A           |
| 25         | RA           | 1982       | C           |
| 25         | RA           | 1991       | U           |
| 25         | RA           | 1992       | G           |
| 25         | RA           | 1993       | U           |
| 25         | RA           | 2023       | G           |
| 25         | RA           | 2031       | A           |
| 25         | RA           | 2032       | G           |
| 25         | RA           | 2033       | A           |
| 25         | RA           | 2043       | C           |
| 25         | RA           | 2055       | C           |
| 25         | RA           | 2056       | G           |
| 25         | RA           | 2059       | A           |
| 25         | RA           | 2060       | A           |
| 25         | RA           | 2061       | G           |
| 25         | RA           | 2062       | A           |
| 25         | RA           | 2069       | G           |
| 25         | RA           | 2093       | G           |
| 25         | RA           | 2099       | U           |
| 25         | RA           | 2100       | G           |
| 25         | RA           | 2107       | C           |
| 25         | RA           | 2111       | C           |
| 25         | RA           | 2113       | U           |
| 25         | RA           | 2114       | A           |
| 25         | RA           | 2115       | G           |
| 25         | RA           | 2116       | G           |
| 25         | RA           | 2117       | A           |
| 25         | RA           | 2126       | A           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2127 | G    |
| 25  | RA    | 2128 | C    |
| 25  | RA    | 2131 | G    |
| 25  | RA    | 2132 | U    |
| 25  | RA    | 2133 | G    |
| 25  | RA    | 2135 | A    |
| 25  | RA    | 2136 | C    |
| 25  | RA    | 2146 | C    |
| 25  | RA    | 2148 | G    |
| 25  | RA    | 2157 | G    |
| 25  | RA    | 2158 | A    |
| 25  | RA    | 2166 | G    |
| 25  | RA    | 2168 | G    |
| 25  | RA    | 2169 | A    |
| 25  | RA    | 2173 | A    |
| 25  | RA    | 2176 | A    |
| 25  | RA    | 2190 | G    |
| 25  | RA    | 2192 | G    |
| 25  | RA    | 2198 | A    |
| 25  | RA    | 2199 | A    |
| 25  | RA    | 2210 | G    |
| 25  | RA    | 2211 | G    |
| 25  | RA    | 2212 | A    |
| 25  | RA    | 2213 | U    |
| 25  | RA    | 2215 | G    |
| 25  | RA    | 2225 | A    |
| 25  | RA    | 2238 | G    |
| 25  | RA    | 2239 | G    |
| 25  | RA    | 2243 | U    |
| 25  | RA    | 2245 | U    |
| 25  | RA    | 2275 | C    |
| 25  | RA    | 2283 | C    |
| 25  | RA    | 2287 | A    |
| 25  | RA    | 2307 | G    |
| 25  | RA    | 2308 | G    |
| 25  | RA    | 2311 | A    |
| 25  | RA    | 2312 | U    |
| 25  | RA    | 2319 | G    |
| 25  | RA    | 2320 | A    |
| 25  | RA    | 2325 | G    |
| 25  | RA    | 2327 | A    |
| 25  | RA    | 2334 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 2336       | A           |
| 25         | RA           | 2345       | G           |
| 25         | RA           | 2346       | A           |
| 25         | RA           | 2347       | C           |
| 25         | RA           | 2350       | C           |
| 25         | RA           | 2354       | G           |
| 25         | RA           | 2379       | G           |
| 25         | RA           | 2383       | G           |
| 25         | RA           | 2385       | C           |
| 25         | RA           | 2391       | G           |
| 25         | RA           | 2392       | A           |
| 25         | RA           | 2394       | C           |
| 25         | RA           | 2402       | C           |
| 25         | RA           | 2403       | C           |
| 25         | RA           | 2406       | U           |
| 25         | RA           | 2410       | G           |
| 25         | RA           | 2423       | U           |
| 25         | RA           | 2424       | C           |
| 25         | RA           | 2425       | A           |
| 25         | RA           | 2429       | G           |
| 25         | RA           | 2430       | A           |
| 25         | RA           | 2435       | A           |
| 25         | RA           | 2439       | A           |
| 25         | RA           | 2440       | C           |
| 25         | RA           | 2441       | C           |
| 25         | RA           | 2445       | G           |
| 25         | RA           | 2448       | A           |
| 25         | RA           | 2469       | A           |
| 25         | RA           | 2470       | G           |
| 25         | RA           | 2474       | C           |
| 25         | RA           | 2475       | C           |
| 25         | RA           | 2482       | G           |
| 25         | RA           | 2494       | G           |
| 25         | RA           | 2502       | G           |
| 25         | RA           | 2505       | G           |
| 25         | RA           | 2519       | U           |
| 25         | RA           | 2520       | C           |
| 25         | RA           | 2529       | G           |
| 25         | RA           | 2542       | A           |
| 25         | RA           | 2543       | G           |
| 25         | RA           | 2554       | U           |
| 25         | RA           | 2567       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 2569    | G    |
| 25  | RA    | 2582    | G    |
| 25  | RA    | 2602    | A    |
| 25  | RA    | 2609    | U    |
| 25  | RA    | 2611    | U    |
| 25  | RA    | 2612    | C    |
| 25  | RA    | 2614    | A    |
| 25  | RA    | 2623    | G    |
| 25  | RA    | 2629    | A    |
| 25  | RA    | 2641    | G    |
| 25  | RA    | 2646    | C    |
| 25  | RA    | 2655    | G    |
| 25  | RA    | 2665    | A    |
| 25  | RA    | 2673    | G    |
| 25  | RA    | 2682    | U    |
| 25  | RA    | 2689    | U    |
| 25  | RA    | 2690    | C    |
| 25  | RA    | 2691    | C    |
| 25  | RA    | 2702    | U    |
| 25  | RA    | 2703    | C    |
| 25  | RA    | 2707    | G    |
| 25  | RA    | 2712    | U    |
| 25  | RA    | 2712(A) | A    |
| 25  | RA    | 2713    | A    |
| 25  | RA    | 2714    | G    |
| 25  | RA    | 2726    | U    |
| 25  | RA    | 2732    | G    |
| 25  | RA    | 2733    | A    |
| 25  | RA    | 2734    | A    |
| 25  | RA    | 2748    | A    |
| 25  | RA    | 2752    | C    |
| 25  | RA    | 2758    | A    |
| 25  | RA    | 2761    | G    |
| 25  | RA    | 2764    | A    |
| 25  | RA    | 2765    | A    |
| 25  | RA    | 2766    | G    |
| 25  | RA    | 2777    | G    |
| 25  | RA    | 2778    | A    |
| 25  | RA    | 2779    | U    |
| 25  | RA    | 2780    | G    |
| 25  | RA    | 2789    | C    |
| 25  | RA    | 2790    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2791 | C    |
| 25  | RA    | 2797 | U    |
| 25  | RA    | 2807 | G    |
| 25  | RA    | 2812 | G    |
| 25  | RA    | 2818 | G    |
| 25  | RA    | 2820 | A    |
| 25  | RA    | 2821 | A    |
| 25  | RA    | 2833 | G    |
| 25  | RA    | 2834 | G    |
| 25  | RA    | 2835 | A    |
| 25  | RA    | 2867 | G    |
| 25  | RA    | 2868 | A    |
| 25  | RA    | 2872 | G    |
| 25  | RA    | 2879 | C    |
| 25  | RA    | 2880 | C    |
| 25  | RA    | 2891 | G    |
| 25  | RA    | 2892 | A    |
| 25  | RA    | 2894 | G    |
| 26  | RB    | 8    | U    |
| 26  | RB    | 9    | G    |
| 26  | RB    | 13   | A    |
| 26  | RB    | 15   | A    |
| 26  | RB    | 16   | G    |
| 26  | RB    | 19   | G    |
| 26  | RB    | 22   | U    |
| 26  | RB    | 25   | A    |
| 26  | RB    | 26   | A    |
| 26  | RB    | 27   | C    |
| 26  | RB    | 32   | C    |
| 26  | RB    | 42   | C    |
| 26  | RB    | 45   | A    |
| 26  | RB    | 47   | C    |
| 26  | RB    | 56   | G    |
| 26  | RB    | 67   | G    |
| 26  | RB    | 73   | A    |
| 26  | RB    | 81   | G    |
| 26  | RB    | 89   | G    |
| 26  | RB    | 105  | G    |
| 26  | RB    | 109  | G    |
| 1   | XA    | 6    | G    |
| 1   | XA    | 7    | G    |
| 1   | XA    | 9    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 22  | G    |
| 1   | XA    | 32  | A    |
| 1   | XA    | 39  | G    |
| 1   | XA    | 47  | C    |
| 1   | XA    | 48  | C    |
| 1   | XA    | 51  | A    |
| 1   | XA    | 54  | C    |
| 1   | XA    | 61  | G    |
| 1   | XA    | 64  | G    |
| 1   | XA    | 65  | U    |
| 1   | XA    | 66  | G    |
| 1   | XA    | 78  | G    |
| 1   | XA    | 79  | G    |
| 1   | XA    | 81  | G    |
| 1   | XA    | 89  | U    |
| 1   | XA    | 90  | C    |
| 1   | XA    | 91  | C    |
| 1   | XA    | 92  | G    |
| 1   | XA    | 95  | G    |
| 1   | XA    | 101 | A    |
| 1   | XA    | 108 | G    |
| 1   | XA    | 116 | A    |
| 1   | XA    | 121 | C    |
| 1   | XA    | 130 | A    |
| 1   | XA    | 144 | G    |
| 1   | XA    | 147 | G    |
| 1   | XA    | 163 | C    |
| 1   | XA    | 172 | A    |
| 1   | XA    | 174 | C    |
| 1   | XA    | 182 | U    |
| 1   | XA    | 190 | G    |
| 1   | XA    | 195 | A    |
| 1   | XA    | 197 | A    |
| 1   | XA    | 201 | C    |
| 1   | XA    | 209 | U    |
| 1   | XA    | 216 | G    |
| 1   | XA    | 222 | U    |
| 1   | XA    | 244 | U    |
| 1   | XA    | 245 | C    |
| 1   | XA    | 247 | G    |
| 1   | XA    | 251 | G    |
| 1   | XA    | 267 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 281 | G    |
| 1   | XA    | 289 | G    |
| 1   | XA    | 306 | G    |
| 1   | XA    | 314 | C    |
| 1   | XA    | 317 | G    |
| 1   | XA    | 321 | A    |
| 1   | XA    | 328 | C    |
| 1   | XA    | 329 | A    |
| 1   | XA    | 332 | G    |
| 1   | XA    | 345 | C    |
| 1   | XA    | 346 | G    |
| 1   | XA    | 347 | G    |
| 1   | XA    | 348 | G    |
| 1   | XA    | 351 | G    |
| 1   | XA    | 352 | C    |
| 1   | XA    | 353 | A    |
| 1   | XA    | 354 | G    |
| 1   | XA    | 356 | A    |
| 1   | XA    | 367 | U    |
| 1   | XA    | 372 | C    |
| 1   | XA    | 373 | A    |
| 1   | XA    | 384 | G    |
| 1   | XA    | 388 | G    |
| 1   | XA    | 389 | A    |
| 1   | XA    | 390 | C    |
| 1   | XA    | 397 | A    |
| 1   | XA    | 398 | C    |
| 1   | XA    | 406 | G    |
| 1   | XA    | 411 | A    |
| 1   | XA    | 412 | A    |
| 1   | XA    | 413 | G    |
| 1   | XA    | 414 | A    |
| 1   | XA    | 421 | U    |
| 1   | XA    | 422 | C    |
| 1   | XA    | 423 | G    |
| 1   | XA    | 424 | G    |
| 1   | XA    | 429 | U    |
| 1   | XA    | 430 | A    |
| 1   | XA    | 442 | C    |
| 1   | XA    | 452 | A    |
| 1   | XA    | 465 | A    |
| 1   | XA    | 466 | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | XA           | 467        | G           |
| 1          | XA           | 482        | A           |
| 1          | XA           | 485        | G           |
| 1          | XA           | 486        | U           |
| 1          | XA           | 496        | A           |
| 1          | XA           | 497        | U           |
| 1          | XA           | 509        | A           |
| 1          | XA           | 510        | A           |
| 1          | XA           | 511        | C           |
| 1          | XA           | 518        | C           |
| 1          | XA           | 527        | G           |
| 1          | XA           | 531        | U           |
| 1          | XA           | 532        | A           |
| 1          | XA           | 533        | A           |
| 1          | XA           | 545        | C           |
| 1          | XA           | 547        | A           |
| 1          | XA           | 548        | G           |
| 1          | XA           | 559        | A           |
| 1          | XA           | 561        | U           |
| 1          | XA           | 564        | C           |
| 1          | XA           | 568        | G           |
| 1          | XA           | 572        | A           |
| 1          | XA           | 573        | A           |
| 1          | XA           | 576        | G           |
| 1          | XA           | 577        | G           |
| 1          | XA           | 579        | G           |
| 1          | XA           | 630        | G           |
| 1          | XA           | 631        | G           |
| 1          | XA           | 633        | G           |
| 1          | XA           | 652        | U           |
| 1          | XA           | 653        | A           |
| 1          | XA           | 665        | A           |
| 1          | XA           | 671        | G           |
| 1          | XA           | 688        | G           |
| 1          | XA           | 702        | A           |
| 1          | XA           | 704        | A           |
| 1          | XA           | 723        | U           |
| 1          | XA           | 731        | G           |
| 1          | XA           | 749        | C           |
| 1          | XA           | 753        | A           |
| 1          | XA           | 754        | C           |
| 1          | XA           | 755        | G           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 774 | G    |
| 1   | XA    | 777 | A    |
| 1   | XA    | 792 | A    |
| 1   | XA    | 793 | U    |
| 1   | XA    | 794 | A    |
| 1   | XA    | 799 | G    |
| 1   | XA    | 813 | U    |
| 1   | XA    | 816 | A    |
| 1   | XA    | 817 | C    |
| 1   | XA    | 818 | G    |
| 1   | XA    | 821 | G    |
| 1   | XA    | 828 | A    |
| 1   | XA    | 836 | G    |
| 1   | XA    | 841 | U    |
| 1   | XA    | 843 | U    |
| 1   | XA    | 848 | C    |
| 1   | XA    | 859 | A    |
| 1   | XA    | 871 | U    |
| 1   | XA    | 872 | A    |
| 1   | XA    | 902 | G    |
| 1   | XA    | 914 | A    |
| 1   | XA    | 926 | G    |
| 1   | XA    | 927 | G    |
| 1   | XA    | 934 | C    |
| 1   | XA    | 935 | A    |
| 1   | XA    | 940 | C    |
| 1   | XA    | 960 | U    |
| 1   | XA    | 961 | U    |
| 1   | XA    | 966 | G    |
| 1   | XA    | 968 | A    |
| 1   | XA    | 969 | A    |
| 1   | XA    | 972 | C    |
| 1   | XA    | 974 | A    |
| 1   | XA    | 975 | A    |
| 1   | XA    | 976 | G    |
| 1   | XA    | 977 | A    |
| 1   | XA    | 980 | C    |
| 1   | XA    | 982 | U    |
| 1   | XA    | 983 | A    |
| 1   | XA    | 991 | U    |
| 1   | XA    | 992 | U    |
| 1   | XA    | 993 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1004    | A    |
| 1   | XA    | 1006    | C    |
| 1   | XA    | 1008    | C    |
| 1   | XA    | 1009    | G    |
| 1   | XA    | 1021    | G    |
| 1   | XA    | 1024    | G    |
| 1   | XA    | 1025    | U    |
| 1   | XA    | 1028    | C    |
| 1   | XA    | 1029    | G    |
| 1   | XA    | 1032(A) | G    |
| 1   | XA    | 1036    | G    |
| 1   | XA    | 1039    | C    |
| 1   | XA    | 1040    | U    |
| 1   | XA    | 1042    | G    |
| 1   | XA    | 1054    | C    |
| 1   | XA    | 1055    | A    |
| 1   | XA    | 1081    | G    |
| 1   | XA    | 1094    | G    |
| 1   | XA    | 1095    | U    |
| 1   | XA    | 1101    | A    |
| 1   | XA    | 1124    | G    |
| 1   | XA    | 1125    | U    |
| 1   | XA    | 1126    | U    |
| 1   | XA    | 1127    | G    |
| 1   | XA    | 1130    | A    |
| 1   | XA    | 1131    | G    |
| 1   | XA    | 1136    | U    |
| 1   | XA    | 1137    | C    |
| 1   | XA    | 1138    | G    |
| 1   | XA    | 1139    | G    |
| 1   | XA    | 1146    | A    |
| 1   | XA    | 1157    | A    |
| 1   | XA    | 1158    | C    |
| 1   | XA    | 1159    | U    |
| 1   | XA    | 1160    | G    |
| 1   | XA    | 1162    | C    |
| 1   | XA    | 1163    | C    |
| 1   | XA    | 1171    | G    |
| 1   | XA    | 1176    | A    |
| 1   | XA    | 1177    | G    |
| 1   | XA    | 1181    | G    |
| 1   | XA    | 1182    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1183    | A    |
| 1   | XA    | 1187    | G    |
| 1   | XA    | 1190    | G    |
| 1   | XA    | 1196    | U    |
| 1   | XA    | 1197    | G    |
| 1   | XA    | 1201    | A    |
| 1   | XA    | 1202    | G    |
| 1   | XA    | 1212    | U    |
| 1   | XA    | 1213    | A    |
| 1   | XA    | 1225    | A    |
| 1   | XA    | 1238    | A    |
| 1   | XA    | 1240    | U    |
| 1   | XA    | 1241    | G    |
| 1   | XA    | 1256    | A    |
| 1   | XA    | 1257    | U    |
| 1   | XA    | 1258    | G    |
| 1   | XA    | 1263    | C    |
| 1   | XA    | 1270    | C    |
| 1   | XA    | 1272    | G    |
| 1   | XA    | 1280    | A    |
| 1   | XA    | 1281    | U    |
| 1   | XA    | 1282    | C    |
| 1   | XA    | 1286    | A    |
| 1   | XA    | 1287    | A    |
| 1   | XA    | 1298    | C    |
| 1   | XA    | 1299    | A    |
| 1   | XA    | 1300    | G    |
| 1   | XA    | 1301    | U    |
| 1   | XA    | 1302    | U    |
| 1   | XA    | 1305    | G    |
| 1   | XA    | 1318    | A    |
| 1   | XA    | 1320    | C    |
| 1   | XA    | 1321    | C    |
| 1   | XA    | 1322    | C    |
| 1   | XA    | 1323    | G    |
| 1   | XA    | 1331    | G    |
| 1   | XA    | 1336    | C    |
| 1   | XA    | 1347    | G    |
| 1   | XA    | 1353    | G    |
| 1   | XA    | 1362(A) | C    |
| 1   | XA    | 1364    | U    |
| 1   | XA    | 1365    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | XA    | 1370 | G    |
| 1   | XA    | 1397 | C    |
| 1   | XA    | 1419 | G    |
| 1   | XA    | 1442 | G    |
| 1   | XA    | 1446 | A    |
| 1   | XA    | 1447 | G    |
| 1   | XA    | 1452 | C    |
| 1   | XA    | 1453 | G    |
| 1   | XA    | 1454 | G    |
| 1   | XA    | 1487 | G    |
| 1   | XA    | 1492 | A    |
| 1   | XA    | 1497 | G    |
| 1   | XA    | 1499 | A    |
| 1   | XA    | 1502 | A    |
| 1   | XA    | 1504 | G    |
| 1   | XA    | 1505 | G    |
| 1   | XA    | 1506 | U    |
| 1   | XA    | 1517 | G    |
| 1   | XA    | 1519 | A    |
| 1   | XA    | 1520 | G    |
| 1   | XA    | 1529 | G    |
| 1   | XA    | 1530 | G    |
| 22  | XV    | 3    | G    |
| 22  | XV    | 4    | G    |
| 22  | XV    | 6    | G    |
| 22  | XV    | 13   | A    |
| 22  | XV    | 15   | C    |
| 22  | XV    | 17   | U    |
| 22  | XV    | 18   | G    |
| 22  | XV    | 19   | G    |
| 22  | XV    | 21   | A    |
| 22  | XV    | 47   | U    |
| 22  | XV    | 48   | C    |
| 22  | XV    | 49   | G    |
| 22  | XV    | 52   | G    |
| 22  | XV    | 54   | U    |
| 22  | XV    | 64   | G    |
| 22  | XV    | 67   | C    |
| 22  | XV    | 76   | A    |
| 23  | XW    | 6    | G    |
| 23  | XW    | 9    | A    |
| 23  | XW    | 11   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | XW    | 14  | A    |
| 23  | XW    | 15  | G    |
| 23  | XW    | 16  | U    |
| 23  | XW    | 17  | C    |
| 23  | XW    | 19  | G    |
| 23  | XW    | 21  | A    |
| 23  | XW    | 39  | U    |
| 23  | XW    | 42  | C    |
| 23  | XW    | 43  | C    |
| 23  | XW    | 44  | G    |
| 23  | XW    | 46  | G    |
| 23  | XW    | 47  | U    |
| 23  | XW    | 57  | G    |
| 23  | XW    | 58  | A    |
| 23  | XW    | 61  | C    |
| 23  | XW    | 70  | G    |
| 23  | XY    | 29  | G    |
| 23  | XY    | 34  | G    |
| 23  | XY    | 36  | A    |
| 23  | XY    | 37  | A    |
| 25  | YA    | 9   | U    |
| 25  | YA    | 15  | G    |
| 25  | YA    | 34  | C    |
| 25  | YA    | 35  | G    |
| 25  | YA    | 46  | C    |
| 25  | YA    | 55  | G    |
| 25  | YA    | 72  | U    |
| 25  | YA    | 74  | A    |
| 25  | YA    | 75  | G    |
| 25  | YA    | 96  | G    |
| 25  | YA    | 101 | G    |
| 25  | YA    | 102 | G    |
| 25  | YA    | 103 | A    |
| 25  | YA    | 118 | A    |
| 25  | YA    | 120 | U    |
| 25  | YA    | 125 | G    |
| 25  | YA    | 131 | G    |
| 25  | YA    | 161 | U    |
| 25  | YA    | 162 | U    |
| 25  | YA    | 181 | A    |
| 25  | YA    | 188 | G    |
| 25  | YA    | 196 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 199    | A    |
| 25  | YA    | 214    | G    |
| 25  | YA    | 215    | G    |
| 25  | YA    | 216    | A    |
| 25  | YA    | 221    | A    |
| 25  | YA    | 222    | A    |
| 25  | YA    | 223    | A    |
| 25  | YA    | 225    | A    |
| 25  | YA    | 228    | A    |
| 25  | YA    | 229    | A    |
| 25  | YA    | 230    | U    |
| 25  | YA    | 232    | G    |
| 25  | YA    | 242    | G    |
| 25  | YA    | 243    | U    |
| 25  | YA    | 248    | G    |
| 25  | YA    | 252    | G    |
| 25  | YA    | 265    | A    |
| 25  | YA    | 266    | G    |
| 25  | YA    | 269    | U    |
| 25  | YA    | 270(L) | U    |
| 25  | YA    | 270(M) | U    |
| 25  | YA    | 270(N) | G    |
| 25  | YA    | 270(P) | C    |
| 25  | YA    | 271(B) | G    |
| 25  | YA    | 271(C) | U    |
| 25  | YA    | 271    | G    |
| 25  | YA    | 274    | G    |
| 25  | YA    | 275    | G    |
| 25  | YA    | 276    | A    |
| 25  | YA    | 278    | A    |
| 25  | YA    | 279    | C    |
| 25  | YA    | 299    | A    |
| 25  | YA    | 300    | A    |
| 25  | YA    | 311    | A    |
| 25  | YA    | 323    | G    |
| 25  | YA    | 324    | A    |
| 25  | YA    | 329    | G    |
| 25  | YA    | 330    | A    |
| 25  | YA    | 332    | A    |
| 25  | YA    | 342    | G    |
| 25  | YA    | 345    | A    |
| 25  | YA    | 352    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | YA    | 363 | G    |
| 25  | YA    | 364 | C    |
| 25  | YA    | 371 | A    |
| 25  | YA    | 372 | G    |
| 25  | YA    | 373 | U    |
| 25  | YA    | 386 | G    |
| 25  | YA    | 387 | U    |
| 25  | YA    | 395 | U    |
| 25  | YA    | 405 | U    |
| 25  | YA    | 406 | G    |
| 25  | YA    | 411 | G    |
| 25  | YA    | 412 | A    |
| 25  | YA    | 428 | A    |
| 25  | YA    | 442 | G    |
| 25  | YA    | 443 | A    |
| 25  | YA    | 444 | C    |
| 25  | YA    | 448 | U    |
| 25  | YA    | 457 | A    |
| 25  | YA    | 470 | A    |
| 25  | YA    | 481 | G    |
| 25  | YA    | 496 | G    |
| 25  | YA    | 504 | U    |
| 25  | YA    | 505 | A    |
| 25  | YA    | 509 | C    |
| 25  | YA    | 512 | G    |
| 25  | YA    | 518 | G    |
| 25  | YA    | 529 | A    |
| 25  | YA    | 531 | C    |
| 25  | YA    | 532 | A    |
| 25  | YA    | 533 | G    |
| 25  | YA    | 537 | C    |
| 25  | YA    | 539 | G    |
| 25  | YA    | 540 | G    |
| 25  | YA    | 546 | C    |
| 25  | YA    | 547 | A    |
| 25  | YA    | 549 | G    |
| 25  | YA    | 563 | G    |
| 25  | YA    | 573 | G    |
| 25  | YA    | 575 | A    |
| 25  | YA    | 588 | U    |
| 25  | YA    | 603 | A    |
| 25  | YA    | 607 | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 609(A) | G    |
| 25  | YA    | 614    | U    |
| 25  | YA    | 615    | G    |
| 25  | YA    | 616    | A    |
| 25  | YA    | 617    | G    |
| 25  | YA    | 620    | G    |
| 25  | YA    | 622    | G    |
| 25  | YA    | 627    | A    |
| 25  | YA    | 637    | A    |
| 25  | YA    | 638    | G    |
| 25  | YA    | 645    | C    |
| 25  | YA    | 646    | A    |
| 25  | YA    | 651    | G    |
| 25  | YA    | 654    | A    |
| 25  | YA    | 654(A) | G    |
| 25  | YA    | 654(B) | C    |
| 25  | YA    | 686    | G    |
| 25  | YA    | 717    | G    |
| 25  | YA    | 722    | A    |
| 25  | YA    | 726    | G    |
| 25  | YA    | 730    | C    |
| 25  | YA    | 734    | A    |
| 25  | YA    | 746    | A    |
| 25  | YA    | 747    | U    |
| 25  | YA    | 753    | C    |
| 25  | YA    | 782    | A    |
| 25  | YA    | 784    | A    |
| 25  | YA    | 785    | G    |
| 25  | YA    | 788    | A    |
| 25  | YA    | 790    | C    |
| 25  | YA    | 792    | G    |
| 25  | YA    | 805    | G    |
| 25  | YA    | 812    | C    |
| 25  | YA    | 819    | A    |
| 25  | YA    | 827    | U    |
| 25  | YA    | 828    | U    |
| 25  | YA    | 847    | U    |
| 25  | YA    | 856    | C    |
| 25  | YA    | 857    | C    |
| 25  | YA    | 859    | G    |
| 25  | YA    | 860    | U    |
| 25  | YA    | 866    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 881        | G           |
| 25         | YA           | 882        | G           |
| 25         | YA           | 884        | C           |
| 25         | YA           | 885        | C           |
| 25         | YA           | 886        | C           |
| 25         | YA           | 888        | C           |
| 25         | YA           | 889        | C           |
| 25         | YA           | 896        | A           |
| 25         | YA           | 897        | C           |
| 25         | YA           | 899        | A           |
| 25         | YA           | 900        | A           |
| 25         | YA           | 901        | A           |
| 25         | YA           | 907        | U           |
| 25         | YA           | 910        | A           |
| 25         | YA           | 914        | C           |
| 25         | YA           | 915        | C           |
| 25         | YA           | 917        | A           |
| 25         | YA           | 932        | G           |
| 25         | YA           | 938        | G           |
| 25         | YA           | 941        | A           |
| 25         | YA           | 945        | A           |
| 25         | YA           | 946        | G           |
| 25         | YA           | 961        | C           |
| 25         | YA           | 974        | G           |
| 25         | YA           | 974(A)     | C           |
| 25         | YA           | 975        | G           |
| 25         | YA           | 980        | A           |
| 25         | YA           | 983        | A           |
| 25         | YA           | 990        | A           |
| 25         | YA           | 991        | C           |
| 25         | YA           | 996        | A           |
| 25         | YA           | 1003       | G           |
| 25         | YA           | 1005       | C           |
| 25         | YA           | 1011       | G           |
| 25         | YA           | 1012       | U           |
| 25         | YA           | 1013       | C           |
| 25         | YA           | 1015       | G           |
| 25         | YA           | 1022       | G           |
| 25         | YA           | 1023       | U           |
| 25         | YA           | 1025       | G           |
| 25         | YA           | 1026       | U           |
| 25         | YA           | 1027       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1033       | U           |
| 25         | YA           | 1045       | A           |
| 25         | YA           | 1046       | A           |
| 25         | YA           | 1050       | A           |
| 25         | YA           | 1054       | A           |
| 25         | YA           | 1055       | G           |
| 25         | YA           | 1059       | G           |
| 25         | YA           | 1060       | U           |
| 25         | YA           | 1061       | U           |
| 25         | YA           | 1066       | U           |
| 25         | YA           | 1067       | A           |
| 25         | YA           | 1068       | G           |
| 25         | YA           | 1070       | A           |
| 25         | YA           | 1071       | G           |
| 25         | YA           | 1076       | C           |
| 25         | YA           | 1077       | A           |
| 25         | YA           | 1078       | U           |
| 25         | YA           | 1079       | C           |
| 25         | YA           | 1082       | U           |
| 25         | YA           | 1083       | U           |
| 25         | YA           | 1084       | A           |
| 25         | YA           | 1085       | A           |
| 25         | YA           | 1086       | A           |
| 25         | YA           | 1088       | A           |
| 25         | YA           | 1089       | G           |
| 25         | YA           | 1095       | A           |
| 25         | YA           | 1096       | A           |
| 25         | YA           | 1097       | U           |
| 25         | YA           | 1099       | G           |
| 25         | YA           | 1103       | A           |
| 25         | YA           | 1104       | C           |
| 25         | YA           | 1110       | G           |
| 25         | YA           | 1111       | A           |
| 25         | YA           | 1122       | G           |
| 25         | YA           | 1131       | G           |
| 25         | YA           | 1135       | C           |
| 25         | YA           | 1136       | G           |
| 25         | YA           | 1139       | G           |
| 25         | YA           | 1142       | U           |
| 25         | YA           | 1142(A)    | A           |
| 25         | YA           | 1170       | G           |
| 25         | YA           | 1173       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1174       | A           |
| 25         | YA           | 1175       | U           |
| 25         | YA           | 1176       | G           |
| 25         | YA           | 1178       | C           |
| 25         | YA           | 1179       | C           |
| 25         | YA           | 1180       | C           |
| 25         | YA           | 1195       | G           |
| 25         | YA           | 1204       | A           |
| 25         | YA           | 1205       | U           |
| 25         | YA           | 1210       | A           |
| 25         | YA           | 1211       | U           |
| 25         | YA           | 1220       | A           |
| 25         | YA           | 1236       | G           |
| 25         | YA           | 1238       | G           |
| 25         | YA           | 1248       | G           |
| 25         | YA           | 1253       | A           |
| 25         | YA           | 1256       | G           |
| 25         | YA           | 1265       | A           |
| 25         | YA           | 1271       | G           |
| 25         | YA           | 1272       | A           |
| 25         | YA           | 1273       | U           |
| 25         | YA           | 1300       | U           |
| 25         | YA           | 1301       | A           |
| 25         | YA           | 1321       | A           |
| 25         | YA           | 1329       | U           |
| 25         | YA           | 1349       | A           |
| 25         | YA           | 1352       | U           |
| 25         | YA           | 1365       | A           |
| 25         | YA           | 1368       | G           |
| 25         | YA           | 1370       | C           |
| 25         | YA           | 1379       | A           |
| 25         | YA           | 1384       | A           |
| 25         | YA           | 1385       | G           |
| 25         | YA           | 1386       | C           |
| 25         | YA           | 1391       | U           |
| 25         | YA           | 1407       | C           |
| 25         | YA           | 1411       | C           |
| 25         | YA           | 1416       | G           |
| 25         | YA           | 1419       | A           |
| 25         | YA           | 1420       | U           |
| 25         | YA           | 1421       | G           |
| 25         | YA           | 1428       | C           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | YA    | 1444(A) | A    |
| 25  | YA    | 1445    | C    |
| 25  | YA    | 1449    | A    |
| 25  | YA    | 1449(A) | G    |
| 25  | YA    | 1455    | G    |
| 25  | YA    | 1458    | C    |
| 25  | YA    | 1460    | A    |
| 25  | YA    | 1461    | G    |
| 25  | YA    | 1467    | C    |
| 25  | YA    | 1471    | A    |
| 25  | YA    | 1482    | U    |
| 25  | YA    | 1483    | G    |
| 25  | YA    | 1493    | C    |
| 25  | YA    | 1497    | U    |
| 25  | YA    | 1506    | C    |
| 25  | YA    | 1507    | A    |
| 25  | YA    | 1508    | A    |
| 25  | YA    | 1510    | A    |
| 25  | YA    | 1511    | A    |
| 25  | YA    | 1514    | U    |
| 25  | YA    | 1522    | G    |
| 25  | YA    | 1534    | G    |
| 25  | YA    | 1535    | U    |
| 25  | YA    | 1536    | A    |
| 25  | YA    | 1537    | C    |
| 25  | YA    | 1543    | A    |
| 25  | YA    | 1544    | C    |
| 25  | YA    | 1545    | A    |
| 25  | YA    | 1547    | C    |
| 25  | YA    | 1554    | A    |
| 25  | YA    | 1558    | A    |
| 25  | YA    | 1559    | G    |
| 25  | YA    | 1566    | A    |
| 25  | YA    | 1569    | A    |
| 25  | YA    | 1578    | U    |
| 25  | YA    | 1579    | A    |
| 25  | YA    | 1580    | A    |
| 25  | YA    | 1585    | C    |
| 25  | YA    | 1586    | A    |
| 25  | YA    | 1592    | C    |
| 25  | YA    | 1598    | C    |
| 25  | YA    | 1599    | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1608       | A           |
| 25         | YA           | 1609       | A           |
| 25         | YA           | 1616       | A           |
| 25         | YA           | 1617       | C           |
| 25         | YA           | 1618       | A           |
| 25         | YA           | 1640       | C           |
| 25         | YA           | 1646       | C           |
| 25         | YA           | 1648       | C           |
| 25         | YA           | 1654       | A           |
| 25         | YA           | 1660       | C           |
| 25         | YA           | 1664       | A           |
| 25         | YA           | 1668       | A           |
| 25         | YA           | 1674       | G           |
| 25         | YA           | 1695       | G           |
| 25         | YA           | 1698       | A           |
| 25         | YA           | 1699       | G           |
| 25         | YA           | 1700       | A           |
| 25         | YA           | 1703       | G           |
| 25         | YA           | 1725       | G           |
| 25         | YA           | 1728       | G           |
| 25         | YA           | 1729       | A           |
| 25         | YA           | 1731       | G           |
| 25         | YA           | 1733       | G           |
| 25         | YA           | 1742       | C           |
| 25         | YA           | 1743       | G           |
| 25         | YA           | 1750       | G           |
| 25         | YA           | 1754       | C           |
| 25         | YA           | 1756       | G           |
| 25         | YA           | 1762       | A           |
| 25         | YA           | 1763       | G           |
| 25         | YA           | 1764       | G           |
| 25         | YA           | 1773       | A           |
| 25         | YA           | 1776       | G           |
| 25         | YA           | 1780       | A           |
| 25         | YA           | 1781       | C           |
| 25         | YA           | 1787       | A           |
| 25         | YA           | 1791       | A           |
| 25         | YA           | 1799       | G           |
| 25         | YA           | 1800       | C           |
| 25         | YA           | 1801       | G           |
| 25         | YA           | 1816       | G           |
| 25         | YA           | 1820       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1829       | A           |
| 25         | YA           | 1835       | G           |
| 25         | YA           | 1847       | A           |
| 25         | YA           | 1850       | G           |
| 25         | YA           | 1858       | G           |
| 25         | YA           | 1869       | G           |
| 25         | YA           | 1870       | C           |
| 25         | YA           | 1872       | A           |
| 25         | YA           | 1878       | G           |
| 25         | YA           | 1882       | C           |
| 25         | YA           | 1888       | G           |
| 25         | YA           | 1889       | A           |
| 25         | YA           | 1896       | G           |
| 25         | YA           | 1903       | G           |
| 25         | YA           | 1919       | A           |
| 25         | YA           | 1930       | G           |
| 25         | YA           | 1931       | U           |
| 25         | YA           | 1937       | A           |
| 25         | YA           | 1939       | U           |
| 25         | YA           | 1955       | U           |
| 25         | YA           | 1956       | U           |
| 25         | YA           | 1963       | U           |
| 25         | YA           | 1964       | G           |
| 25         | YA           | 1967       | C           |
| 25         | YA           | 1969       | A           |
| 25         | YA           | 1971       | A           |
| 25         | YA           | 1972       | A           |
| 25         | YA           | 1981       | A           |
| 25         | YA           | 1982       | C           |
| 25         | YA           | 1991       | U           |
| 25         | YA           | 1992       | G           |
| 25         | YA           | 1993       | U           |
| 25         | YA           | 2020       | A           |
| 25         | YA           | 2023       | G           |
| 25         | YA           | 2031       | A           |
| 25         | YA           | 2033       | A           |
| 25         | YA           | 2039       | C           |
| 25         | YA           | 2043       | C           |
| 25         | YA           | 2049       | G           |
| 25         | YA           | 2052       | G           |
| 25         | YA           | 2055       | C           |
| 25         | YA           | 2056       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2059 | A    |
| 25  | YA    | 2060 | A    |
| 25  | YA    | 2061 | G    |
| 25  | YA    | 2062 | A    |
| 25  | YA    | 2063 | C    |
| 25  | YA    | 2069 | G    |
| 25  | YA    | 2093 | G    |
| 25  | YA    | 2099 | U    |
| 25  | YA    | 2100 | G    |
| 25  | YA    | 2111 | C    |
| 25  | YA    | 2112 | G    |
| 25  | YA    | 2113 | U    |
| 25  | YA    | 2114 | A    |
| 25  | YA    | 2115 | G    |
| 25  | YA    | 2116 | G    |
| 25  | YA    | 2117 | A    |
| 25  | YA    | 2119 | A    |
| 25  | YA    | 2120 | G    |
| 25  | YA    | 2126 | A    |
| 25  | YA    | 2127 | G    |
| 25  | YA    | 2128 | C    |
| 25  | YA    | 2131 | G    |
| 25  | YA    | 2132 | U    |
| 25  | YA    | 2133 | G    |
| 25  | YA    | 2136 | C    |
| 25  | YA    | 2146 | C    |
| 25  | YA    | 2148 | G    |
| 25  | YA    | 2158 | A    |
| 25  | YA    | 2166 | G    |
| 25  | YA    | 2168 | G    |
| 25  | YA    | 2173 | A    |
| 25  | YA    | 2176 | A    |
| 25  | YA    | 2178 | C    |
| 25  | YA    | 2190 | G    |
| 25  | YA    | 2192 | G    |
| 25  | YA    | 2198 | A    |
| 25  | YA    | 2210 | G    |
| 25  | YA    | 2211 | G    |
| 25  | YA    | 2212 | A    |
| 25  | YA    | 2213 | U    |
| 25  | YA    | 2215 | G    |
| 25  | YA    | 2225 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2238 | G    |
| 25  | YA    | 2239 | G    |
| 25  | YA    | 2243 | U    |
| 25  | YA    | 2246 | G    |
| 25  | YA    | 2275 | C    |
| 25  | YA    | 2280 | G    |
| 25  | YA    | 2283 | C    |
| 25  | YA    | 2287 | A    |
| 25  | YA    | 2288 | A    |
| 25  | YA    | 2305 | A    |
| 25  | YA    | 2307 | G    |
| 25  | YA    | 2308 | G    |
| 25  | YA    | 2311 | A    |
| 25  | YA    | 2319 | G    |
| 25  | YA    | 2320 | A    |
| 25  | YA    | 2325 | G    |
| 25  | YA    | 2334 | G    |
| 25  | YA    | 2336 | A    |
| 25  | YA    | 2342 | C    |
| 25  | YA    | 2346 | A    |
| 25  | YA    | 2347 | C    |
| 25  | YA    | 2350 | C    |
| 25  | YA    | 2377 | A    |
| 25  | YA    | 2383 | G    |
| 25  | YA    | 2385 | C    |
| 25  | YA    | 2392 | A    |
| 25  | YA    | 2402 | C    |
| 25  | YA    | 2403 | C    |
| 25  | YA    | 2406 | U    |
| 25  | YA    | 2410 | G    |
| 25  | YA    | 2423 | U    |
| 25  | YA    | 2425 | A    |
| 25  | YA    | 2429 | G    |
| 25  | YA    | 2430 | A    |
| 25  | YA    | 2434 | A    |
| 25  | YA    | 2435 | A    |
| 25  | YA    | 2439 | A    |
| 25  | YA    | 2440 | C    |
| 25  | YA    | 2441 | C    |
| 25  | YA    | 2448 | A    |
| 25  | YA    | 2450 | A    |
| 25  | YA    | 2469 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | YA    | 2470    | G    |
| 25  | YA    | 2471    | C    |
| 25  | YA    | 2474    | C    |
| 25  | YA    | 2475    | C    |
| 25  | YA    | 2476    | A    |
| 25  | YA    | 2484    | G    |
| 25  | YA    | 2494    | G    |
| 25  | YA    | 2498    | C    |
| 25  | YA    | 2502    | G    |
| 25  | YA    | 2505    | G    |
| 25  | YA    | 2518    | A    |
| 25  | YA    | 2524    | G    |
| 25  | YA    | 2529    | G    |
| 25  | YA    | 2542    | A    |
| 25  | YA    | 2543    | G    |
| 25  | YA    | 2554    | U    |
| 25  | YA    | 2562    | U    |
| 25  | YA    | 2566    | A    |
| 25  | YA    | 2567    | G    |
| 25  | YA    | 2586    | C    |
| 25  | YA    | 2602    | A    |
| 25  | YA    | 2609    | U    |
| 25  | YA    | 2611    | U    |
| 25  | YA    | 2612    | C    |
| 25  | YA    | 2621    | A    |
| 25  | YA    | 2629    | A    |
| 25  | YA    | 2632    | A    |
| 25  | YA    | 2655    | G    |
| 25  | YA    | 2656    | U    |
| 25  | YA    | 2665    | A    |
| 25  | YA    | 2673    | G    |
| 25  | YA    | 2682    | U    |
| 25  | YA    | 2689    | U    |
| 25  | YA    | 2690    | C    |
| 25  | YA    | 2702    | U    |
| 25  | YA    | 2703    | C    |
| 25  | YA    | 2712    | U    |
| 25  | YA    | 2712(A) | A    |
| 25  | YA    | 2713    | A    |
| 25  | YA    | 2714    | G    |
| 25  | YA    | 2720    | U    |
| 25  | YA    | 2726    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2733 | A    |
| 25  | YA    | 2744 | G    |
| 25  | YA    | 2748 | A    |
| 25  | YA    | 2752 | C    |
| 25  | YA    | 2757 | A    |
| 25  | YA    | 2758 | A    |
| 25  | YA    | 2761 | G    |
| 25  | YA    | 2764 | A    |
| 25  | YA    | 2765 | A    |
| 25  | YA    | 2766 | G    |
| 25  | YA    | 2777 | G    |
| 25  | YA    | 2778 | A    |
| 25  | YA    | 2779 | U    |
| 25  | YA    | 2780 | G    |
| 25  | YA    | 2789 | C    |
| 25  | YA    | 2790 | A    |
| 25  | YA    | 2791 | C    |
| 25  | YA    | 2797 | U    |
| 25  | YA    | 2799 | A    |
| 25  | YA    | 2807 | G    |
| 25  | YA    | 2808 | U    |
| 25  | YA    | 2818 | G    |
| 25  | YA    | 2820 | A    |
| 25  | YA    | 2821 | A    |
| 25  | YA    | 2823 | A    |
| 25  | YA    | 2833 | G    |
| 25  | YA    | 2834 | G    |
| 25  | YA    | 2835 | A    |
| 25  | YA    | 2867 | G    |
| 25  | YA    | 2868 | A    |
| 25  | YA    | 2872 | G    |
| 25  | YA    | 2873 | A    |
| 25  | YA    | 2880 | C    |
| 25  | YA    | 2891 | G    |
| 25  | YA    | 2892 | A    |
| 25  | YA    | 2893 | G    |
| 25  | YA    | 2894 | G    |
| 26  | YB    | 8    | U    |
| 26  | YB    | 9    | G    |
| 26  | YB    | 13   | A    |
| 26  | YB    | 15   | A    |
| 26  | YB    | 16   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | YB    | 21  | G    |
| 26  | YB    | 22  | U    |
| 26  | YB    | 25  | A    |
| 26  | YB    | 32  | C    |
| 26  | YB    | 40  | U    |
| 26  | YB    | 41  | U    |
| 26  | YB    | 42  | C    |
| 26  | YB    | 45  | A    |
| 26  | YB    | 47  | C    |
| 26  | YB    | 52  | A    |
| 26  | YB    | 53  | A    |
| 26  | YB    | 56  | G    |
| 26  | YB    | 67  | G    |
| 26  | YB    | 73  | A    |
| 26  | YB    | 89  | G    |
| 26  | YB    | 109 | G    |

All (199) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 5   | U    |
| 1   | QA    | 31  | G    |
| 1   | QA    | 64  | G    |
| 1   | QA    | 115 | G    |
| 1   | QA    | 119 | A    |
| 1   | QA    | 181 | G    |
| 1   | QA    | 243 | A    |
| 1   | QA    | 244 | U    |
| 1   | QA    | 250 | A    |
| 1   | QA    | 266 | G    |
| 1   | QA    | 328 | C    |
| 1   | QA    | 410 | G    |
| 1   | QA    | 412 | A    |
| 1   | QA    | 429 | U    |
| 1   | QA    | 481 | G    |
| 1   | QA    | 484 | G    |
| 1   | QA    | 485 | G    |
| 1   | QA    | 509 | A    |
| 1   | QA    | 533 | A    |
| 1   | QA    | 687 | A    |
| 1   | QA    | 701 | C    |
| 1   | QA    | 703 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 753    | A    |
| 1   | QA    | 792    | A    |
| 1   | QA    | 812    | C    |
| 1   | QA    | 913    | A    |
| 1   | QA    | 934    | C    |
| 1   | QA    | 960    | U    |
| 1   | QA    | 992    | U    |
| 1   | QA    | 1027   | C    |
| 1   | QA    | 1064   | G    |
| 1   | QA    | 1065   | U    |
| 1   | QA    | 1200   | C    |
| 1   | QA    | 1201   | A    |
| 1   | QA    | 1285   | A    |
| 1   | QA    | 1297   | C    |
| 1   | QA    | 1336   | C    |
| 1   | QA    | 1346   | A    |
| 1   | QA    | 1347   | G    |
| 1   | QA    | 1446   | A    |
| 1   | QA    | 1498   | U    |
| 1   | QA    | 1503   | A    |
| 1   | QA    | 1528   | U    |
| 22  | QV    | 53     | G    |
| 25  | RA    | 27     | G    |
| 25  | RA    | 74     | A    |
| 25  | RA    | 99     | U    |
| 25  | RA    | 102    | G    |
| 25  | RA    | 195    | A    |
| 25  | RA    | 205    | G    |
| 25  | RA    | 221    | A    |
| 25  | RA    | 222    | A    |
| 25  | RA    | 227    | A    |
| 25  | RA    | 229    | A    |
| 25  | RA    | 242    | G    |
| 25  | RA    | 271(B) | G    |
| 25  | RA    | 271(C) | U    |
| 25  | RA    | 345    | A    |
| 25  | RA    | 372    | G    |
| 25  | RA    | 404    | C    |
| 25  | RA    | 503    | A    |
| 25  | RA    | 512    | G    |
| 25  | RA    | 587    | C    |
| 25  | RA    | 637    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 846        | C           |
| 25         | RA           | 856        | C           |
| 25         | RA           | 859        | G           |
| 25         | RA           | 974(A)     | C           |
| 25         | RA           | 1012       | U           |
| 25         | RA           | 1022       | G           |
| 25         | RA           | 1026       | U           |
| 25         | RA           | 1045       | A           |
| 25         | RA           | 1078       | U           |
| 25         | RA           | 1085       | A           |
| 25         | RA           | 1130       | U           |
| 25         | RA           | 1178       | C           |
| 25         | RA           | 1204       | A           |
| 25         | RA           | 1210       | A           |
| 25         | RA           | 1312       | U           |
| 25         | RA           | 1427       | A           |
| 25         | RA           | 1558       | A           |
| 25         | RA           | 1653       | G           |
| 25         | RA           | 1694       | C           |
| 25         | RA           | 1799       | G           |
| 25         | RA           | 1819       | A           |
| 25         | RA           | 1930       | G           |
| 25         | RA           | 1980       | G           |
| 25         | RA           | 1992       | G           |
| 25         | RA           | 2060       | A           |
| 25         | RA           | 2126       | A           |
| 25         | RA           | 2405       | G           |
| 25         | RA           | 2439       | A           |
| 25         | RA           | 2481       | G           |
| 25         | RA           | 2518       | A           |
| 25         | RA           | 2566       | A           |
| 25         | RA           | 2610       | C           |
| 25         | RA           | 2689       | U           |
| 25         | RA           | 2712       | U           |
| 25         | RA           | 2776       | A           |
| 25         | RA           | 2832       | U           |
| 25         | RA           | 2867       | G           |
| 26         | RB           | 66         | A           |
| 1          | XA           | 31         | G           |
| 1          | XA           | 60         | A           |
| 1          | XA           | 64         | G           |
| 1          | XA           | 78         | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | XA           | 89         | U           |
| 1          | XA           | 115        | G           |
| 1          | XA           | 181        | G           |
| 1          | XA           | 243        | A           |
| 1          | XA           | 244        | U           |
| 1          | XA           | 250        | A           |
| 1          | XA           | 266        | G           |
| 1          | XA           | 328        | C           |
| 1          | XA           | 345        | C           |
| 1          | XA           | 410        | G           |
| 1          | XA           | 412        | A           |
| 1          | XA           | 428        | G           |
| 1          | XA           | 429        | U           |
| 1          | XA           | 481        | G           |
| 1          | XA           | 484        | G           |
| 1          | XA           | 485        | G           |
| 1          | XA           | 509        | A           |
| 1          | XA           | 532        | A           |
| 1          | XA           | 560        | U           |
| 1          | XA           | 687        | A           |
| 1          | XA           | 703        | G           |
| 1          | XA           | 753        | A           |
| 1          | XA           | 812        | C           |
| 1          | XA           | 913        | A           |
| 1          | XA           | 991        | U           |
| 1          | XA           | 992        | U           |
| 1          | XA           | 1027       | C           |
| 1          | XA           | 1126       | U           |
| 1          | XA           | 1200       | C           |
| 1          | XA           | 1285       | A           |
| 1          | XA           | 1297       | C           |
| 1          | XA           | 1446       | A           |
| 1          | XA           | 1498       | U           |
| 1          | XA           | 1503       | A           |
| 22         | XV           | 53         | G           |
| 25         | YA           | 99         | U           |
| 25         | YA           | 102        | G           |
| 25         | YA           | 195        | A           |
| 25         | YA           | 221        | A           |
| 25         | YA           | 222        | A           |
| 25         | YA           | 229        | A           |
| 25         | YA           | 242        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 271(B)     | G           |
| 25         | YA           | 278        | A           |
| 25         | YA           | 372        | G           |
| 25         | YA           | 404        | C           |
| 25         | YA           | 503        | A           |
| 25         | YA           | 508        | G           |
| 25         | YA           | 587        | C           |
| 25         | YA           | 637        | A           |
| 25         | YA           | 653        | A           |
| 25         | YA           | 654        | A           |
| 25         | YA           | 752        | A           |
| 25         | YA           | 846        | C           |
| 25         | YA           | 856        | C           |
| 25         | YA           | 859        | G           |
| 25         | YA           | 896        | A           |
| 25         | YA           | 974(A)     | C           |
| 25         | YA           | 1012       | U           |
| 25         | YA           | 1022       | G           |
| 25         | YA           | 1026       | U           |
| 25         | YA           | 1045       | A           |
| 25         | YA           | 1078       | U           |
| 25         | YA           | 1085       | A           |
| 25         | YA           | 1109       | C           |
| 25         | YA           | 1130       | U           |
| 25         | YA           | 1178       | C           |
| 25         | YA           | 1210       | A           |
| 25         | YA           | 1427       | A           |
| 25         | YA           | 1558       | A           |
| 25         | YA           | 1653       | G           |
| 25         | YA           | 1694       | C           |
| 25         | YA           | 1698       | A           |
| 25         | YA           | 1799       | G           |
| 25         | YA           | 1819       | A           |
| 25         | YA           | 1929       | G           |
| 25         | YA           | 1930       | G           |
| 25         | YA           | 1955       | U           |
| 25         | YA           | 1992       | G           |
| 25         | YA           | 2126       | A           |
| 25         | YA           | 2439       | A           |
| 25         | YA           | 2566       | A           |
| 25         | YA           | 2610       | C           |
| 25         | YA           | 2655       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2681 | C    |
| 25  | YA    | 2689 | U    |
| 25  | YA    | 2712 | U    |
| 25  | YA    | 2719 | G    |
| 25  | YA    | 2756 | U    |
| 25  | YA    | 2776 | A    |
| 25  | YA    | 2832 | U    |
| 25  | YA    | 2867 | G    |
| 26  | YB    | 66   | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 704 ligands modelled in this entry, 702 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | PAR  | XA    | 1672 | -    | 45,45,45     | 1.53 | 7 (15%)  | 64,67,67    | 1.26 | 5 (7%)   |
| 58  | PAR  | QA    | 1667 | -    | 45,45,45     | 1.55 | 7 (15%)  | 64,67,67    | 1.17 | 5 (7%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 58  | PAR  | XA    | 1672 | -    | -       | 5/18/94/94 | 0/4/4/4 |
| 58  | PAR  | QA    | 1667 | -    | -       | 5/18/94/94 | 0/4/4/4 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58  | QA    | 1667 | PAR  | C64-C54 | 5.11 | 1.59        | 1.52     |
| 58  | XA    | 1672 | PAR  | C64-C54 | 5.01 | 1.58        | 1.52     |
| 58  | QA    | 1667 | PAR  | C52-C42 | 3.12 | 1.58        | 1.52     |
| 58  | XA    | 1672 | PAR  | C52-C42 | 3.05 | 1.58        | 1.52     |
| 58  | XA    | 1672 | PAR  | O54-C14 | 3.01 | 1.49        | 1.41     |
| 58  | QA    | 1667 | PAR  | O54-C14 | 2.93 | 1.49        | 1.41     |
| 58  | XA    | 1672 | PAR  | C11-C21 | 2.78 | 1.57        | 1.52     |
| 58  | QA    | 1667 | PAR  | C11-C21 | 2.71 | 1.57        | 1.52     |
| 58  | QA    | 1667 | PAR  | O51-C11 | 2.55 | 1.48        | 1.41     |
| 58  | XA    | 1672 | PAR  | O51-C11 | 2.54 | 1.48        | 1.41     |
| 58  | XA    | 1672 | PAR  | C14-C24 | 2.31 | 1.56        | 1.52     |
| 58  | QA    | 1667 | PAR  | C31-C21 | 2.29 | 1.56        | 1.53     |
| 58  | QA    | 1667 | PAR  | C14-C24 | 2.18 | 1.56        | 1.52     |
| 58  | XA    | 1672 | PAR  | C31-C21 | 2.12 | 1.56        | 1.53     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 58  | XA    | 1672 | PAR  | C14-O54-C54 | 4.10 | 121.73      | 113.69   |
| 58  | QA    | 1667 | PAR  | C14-O54-C54 | 4.04 | 121.62      | 113.69   |
| 58  | QA    | 1667 | PAR  | O52-C13-C23 | 3.57 | 115.35      | 107.96   |
| 58  | QA    | 1667 | PAR  | O33-C14-C24 | 3.49 | 114.23      | 108.22   |
| 58  | XA    | 1672 | PAR  | O54-C54-C64 | 3.38 | 112.29      | 106.01   |
| 58  | XA    | 1672 | PAR  | O33-C14-C24 | 3.26 | 113.83      | 108.22   |
| 58  | QA    | 1667 | PAR  | O54-C54-C64 | 3.19 | 111.95      | 106.01   |
| 58  | XA    | 1672 | PAR  | O52-C13-C23 | 3.04 | 114.27      | 107.96   |
| 58  | XA    | 1672 | PAR  | C11-O51-C51 | 2.43 | 118.46      | 113.69   |
| 58  | QA    | 1667 | PAR  | C11-O51-C51 | 2.03 | 117.67      | 113.69   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 58  | XA    | 1672 | PAR  | O43-C43-C53-O53 |
| 58  | XA    | 1672 | PAR  | C33-C43-C53-O53 |
| 58  | QA    | 1667 | PAR  | C33-C43-C53-O53 |

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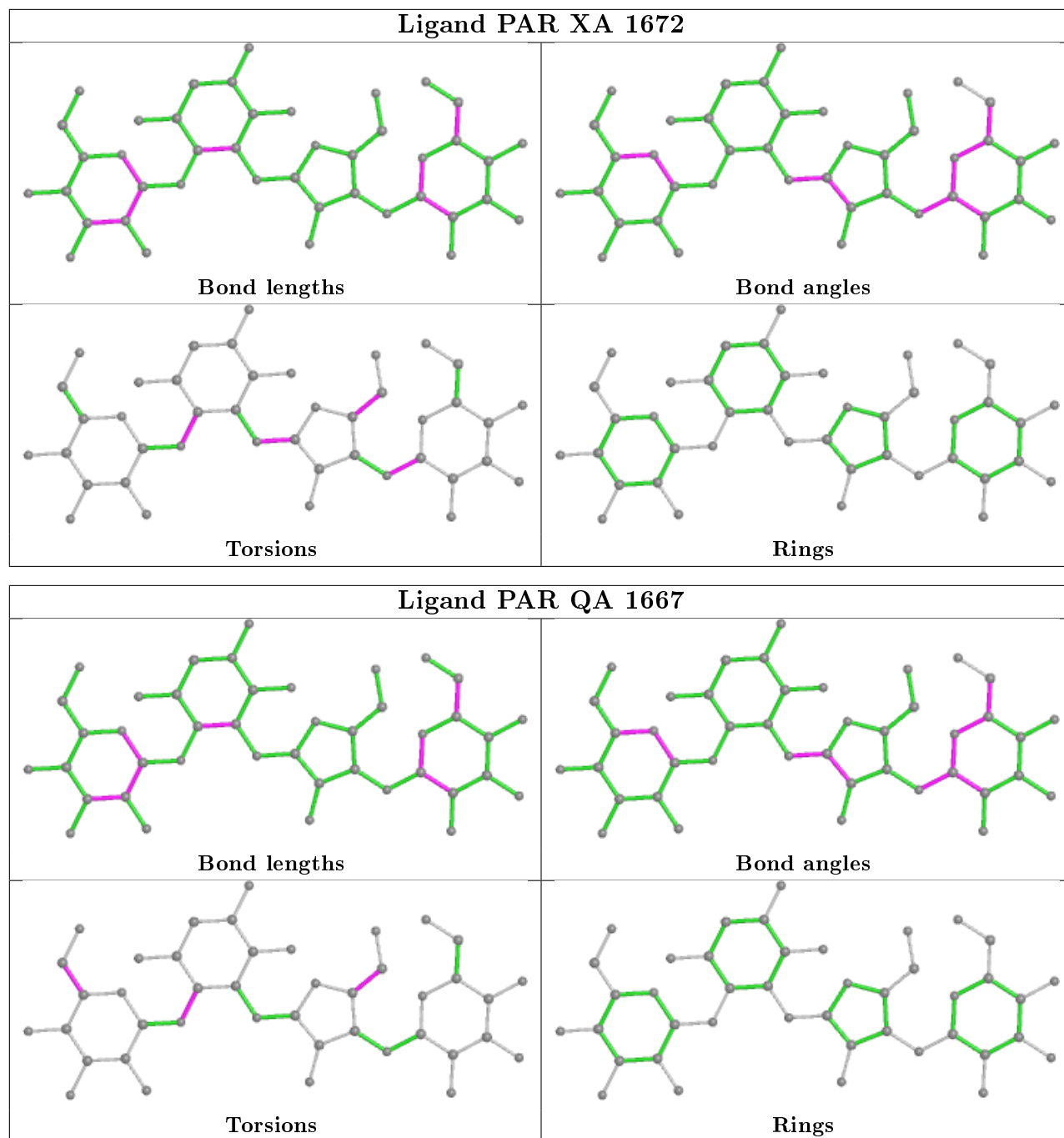
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 58  | QA    | 1667 | PAR  | O43-C43-C53-O53 |
| 58  | QA    | 1667 | PAR  | C41-C51-C61-O61 |
| 58  | QA    | 1667 | PAR  | O51-C51-C61-O61 |
| 58  | XA    | 1672 | PAR  | C52-C42-O11-C11 |
| 58  | XA    | 1672 | PAR  | C23-C13-O52-C52 |
| 58  | XA    | 1672 | PAR  | C24-C14-O33-C33 |
| 58  | QA    | 1667 | PAR  | C52-C42-O11-C11 |

There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | XA    | 1672 | PAR  | 4       | 0            |
| 58  | QA    | 1667 | PAR  | 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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   | QA    | 1500/1522 (98%) | 0.27   | 61 (4%) 37 24 | 68, 102, 211, 576     | 0     |
| 1   | XA    | 1500/1522 (98%) | 0.22   | 50 (3%) 46 31 | 57, 88, 196, 440      | 0     |
| 2   | QB    | 237/256 (92%)   | 0.44   | 26 (10%) 5 3  | 106, 186, 344, 418    | 0     |
| 2   | XB    | 237/256 (92%)   | 0.15   | 13 (5%) 25 15 | 88, 156, 283, 529     | 0     |
| 3   | QC    | 205/239 (85%)   | 0.57   | 22 (10%) 6 3  | 103, 172, 294, 429    | 0     |
| 3   | XC    | 205/239 (85%)   | 0.13   | 9 (4%) 34 21  | 80, 124, 195, 316     | 0     |
| 4   | QD    | 208/209 (99%)   | -0.04  | 2 (0%) 82 70  | 85, 114, 192, 458     | 0     |
| 4   | XD    | 208/209 (99%)   | -0.00  | 3 (1%) 75 61  | 71, 109, 190, 368     | 0     |
| 5   | QE    | 151/162 (93%)   | 0.14   | 6 (3%) 38 25  | 90, 128, 201, 260     | 0     |
| 5   | XE    | 151/162 (93%)   | -0.01  | 2 (1%) 77 63  | 72, 101, 185, 236     | 0     |
| 6   | QF    | 101/101 (100%)  | -0.02  | 2 (1%) 65 49  | 80, 109, 175, 310     | 0     |
| 6   | XF    | 101/101 (100%)  | 0.12   | 5 (4%) 28 18  | 73, 107, 161, 559     | 0     |
| 7   | QG    | 155/156 (99%)   | 0.20   | 10 (6%) 18 11 | 83, 150, 262, 534     | 0     |
| 7   | XG    | 155/156 (99%)   | -0.03  | 5 (3%) 47 32  | 76, 129, 209, 334     | 0     |
| 8   | QH    | 138/138 (100%)  | -0.05  | 0 100 100     | 92, 133, 195, 285     | 0     |
| 8   | XH    | 138/138 (100%)  | -0.09  | 0 100 100     | 80, 113, 165, 331     | 0     |
| 9   | QI    | 127/128 (99%)   | 0.56   | 15 (11%) 4 3  | 96, 189, 303, 476     | 0     |
| 9   | XI    | 127/128 (99%)   | 0.32   | 9 (7%) 16 9   | 76, 153, 232, 396     | 0     |
| 10  | QJ    | 99/105 (94%)    | 0.71   | 13 (13%) 3 2  | 107, 196, 431, 583    | 0     |
| 10  | XJ    | 99/105 (94%)    | 0.55   | 10 (10%) 7 4  | 85, 164, 316, 369     | 0     |
| 11  | QK    | 119/129 (92%)   | 0.16   | 7 (5%) 22 13  | 77, 112, 201, 335     | 0     |
| 11  | XK    | 119/129 (92%)   | 0.02   | 4 (3%) 45 30  | 67, 105, 181, 251     | 0     |
| 12  | QL    | 125/132 (94%)   | 0.04   | 3 (2%) 59 42  | 79, 101, 176, 309     | 0     |
| 12  | XL    | 125/132 (94%)   | -0.01  | 4 (3%) 47 32  | 55, 78, 146, 341      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | QM    | 121/126 (96%)   | 0.09   | 2 (1%) 70 55   | 101, 160, 265, 447    | 0     |
| 13  | XM    | 121/126 (96%)   | -0.02  | 2 (1%) 70 55   | 78, 126, 200, 488     | 0     |
| 14  | QN    | 60/61 (98%)     | 0.40   | 3 (5%) 28 18   | 117, 157, 211, 250    | 0     |
| 14  | XN    | 60/61 (98%)     | -0.01  | 0 100 100      | 89, 106, 151, 194     | 0     |
| 15  | QO    | 88/89 (98%)     | 0.08   | 3 (3%) 45 30   | 77, 113, 167, 241     | 0     |
| 15  | XO    | 88/89 (98%)     | -0.02  | 1 (1%) 80 68   | 69, 101, 153, 171     | 0     |
| 16  | QP    | 84/88 (95%)     | 0.09   | 2 (2%) 59 42   | 85, 102, 164, 241     | 0     |
| 16  | XP    | 84/88 (95%)     | 0.09   | 2 (2%) 59 42   | 87, 111, 187, 400     | 0     |
| 17  | QQ    | 100/105 (95%)   | 0.03   | 0 100 100      | 82, 107, 157, 336     | 0     |
| 17  | XQ    | 100/105 (95%)   | 0.01   | 1 (1%) 82 70   | 71, 105, 171, 330     | 0     |
| 18  | QR    | 70/88 (79%)     | -0.00  | 3 (4%) 35 22   | 83, 114, 185, 205     | 0     |
| 18  | XR    | 70/88 (79%)     | 0.04   | 1 (1%) 75 61   | 77, 112, 187, 227     | 0     |
| 19  | QS    | 84/93 (90%)     | 0.38   | 4 (4%) 30 19   | 109, 181, 257, 381    | 0     |
| 19  | XS    | 84/93 (90%)     | 0.07   | 5 (5%) 21 12   | 80, 133, 207, 286     | 0     |
| 20  | QT    | 99/106 (93%)    | 0.10   | 4 (4%) 38 25   | 87, 122, 208, 237     | 0     |
| 20  | XT    | 99/106 (93%)    | 0.22   | 2 (2%) 65 49   | 87, 136, 211, 236     | 0     |
| 21  | QU    | 25/27 (92%)     | 1.05   | 5 (20%) 1 0    | 112, 155, 238, 264    | 0     |
| 21  | XU    | 25/27 (92%)     | 0.37   | 2 (8%) 12 7    | 102, 128, 202, 210    | 0     |
| 22  | QV    | 77/77 (100%)    | 0.46   | 6 (7%) 13 8    | 91, 114, 175, 228     | 0     |
| 22  | XV    | 77/77 (100%)    | 0.15   | 4 (5%) 27 17   | 70, 91, 164, 210      | 0     |
| 23  | QW    | 76/76 (100%)    | 2.07   | 34 (44%) 0 0   | 91, 205, 292, 361     | 0     |
| 23  | QY    | 17/76 (22%)     | 1.59   | 9 (52%) 0 0    | 120, 132, 201, 212    | 0     |
| 23  | XW    | 76/76 (100%)    | 2.27   | 33 (43%) 0 0   | 88, 196, 373, 402     | 0     |
| 23  | XY    | 17/76 (22%)     | 0.66   | 1 (5%) 22 13   | 94, 101, 177, 187     | 0     |
| 24  | QX    | 10/24 (41%)     | 1.59   | 3 (30%) 0 0    | 102, 106, 257, 377    | 0     |
| 24  | XX    | 10/24 (41%)     | 1.88   | 5 (50%) 0 0    | 94, 99, 237, 284      | 0     |
| 25  | RA    | 2882/2915 (98%) | 0.37   | 190 (6%) 18 10 | 53, 82, 254, 563      | 0     |
| 25  | YA    | 2883/2915 (98%) | 0.19   | 127 (4%) 34 21 | 39, 64, 217, 437      | 0     |
| 26  | RB    | 120/122 (98%)   | 0.65   | 14 (11%) 4 3   | 119, 162, 204, 242    | 0     |
| 26  | YB    | 120/122 (98%)   | 0.18   | 1 (0%) 86 75   | 71, 106, 119, 200     | 0     |
| 27  | RD    | 272/276 (98%)   | -0.27  | 1 (0%) 92 86   | 54, 74, 127, 183      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27  | YD    | 272/276 (98%)  | -0.30  | 1 (0%) 92 86  | 40, 66, 120, 213      | 0     |
| 28  | RE    | 205/206 (99%)  | 0.06   | 8 (3%) 39 25  | 55, 94, 188, 447      | 0     |
| 28  | YE    | 205/206 (99%)  | 0.02   | 6 (2%) 51 35  | 43, 78, 167, 453      | 0     |
| 29  | RF    | 202/210 (96%)  | -0.10  | 2 (0%) 82 70  | 54, 110, 191, 469     | 0     |
| 29  | YF    | 202/210 (96%)  | -0.25  | 4 (1%) 65 49  | 39, 71, 138, 248      | 0     |
| 30  | RG    | 181/182 (99%)  | 0.54   | 16 (8%) 10 6  | 122, 192, 303, 490    | 0     |
| 30  | YG    | 181/182 (99%)  | 0.07   | 2 (1%) 80 68  | 82, 117, 183, 391     | 0     |
| 31  | RH    | 170/180 (94%)  | 0.75   | 24 (14%) 2 2  | 113, 199, 359, 517    | 0     |
| 31  | YH    | 170/180 (94%)  | 0.15   | 5 (2%) 51 35  | 65, 114, 180, 363     | 0     |
| 32  | RI    | 146/148 (98%)  | 0.23   | 10 (6%) 17 10 | 73, 155, 265, 529     | 0     |
| 32  | YI    | 146/148 (98%)  | 0.05   | 4 (2%) 54 38  | 62, 143, 271, 559     | 0     |
| 33  | RN    | 138/140 (98%)  | -0.07  | 3 (2%) 62 45  | 64, 111, 186, 302     | 0     |
| 33  | YN    | 138/140 (98%)  | -0.28  | 2 (1%) 75 61  | 49, 78, 167, 266      | 0     |
| 34  | RO    | 122/122 (100%) | -0.25  | 0 100 100     | 63, 94, 139, 155      | 0     |
| 34  | YO    | 122/122 (100%) | -0.28  | 0 100 100     | 51, 68, 115, 146      | 0     |
| 35  | RP    | 150/150 (100%) | 0.10   | 8 (5%) 26 16  | 61, 122, 202, 369     | 0     |
| 35  | YP    | 150/150 (100%) | -0.20  | 1 (0%) 87 78  | 42, 81, 157, 361      | 0     |
| 36  | RQ    | 141/141 (100%) | 0.18   | 7 (4%) 28 18  | 80, 122, 205, 332     | 0     |
| 36  | YQ    | 141/141 (100%) | -0.21  | 3 (2%) 63 48  | 56, 73, 148, 430      | 0     |
| 37  | RR    | 118/118 (100%) | -0.20  | 1 (0%) 86 75  | 61, 86, 134, 160      | 0     |
| 37  | YR    | 118/118 (100%) | -0.18  | 1 (0%) 86 75  | 51, 71, 120, 207      | 0     |
| 38  | RS    | 111/112 (99%)  | 0.23   | 3 (2%) 54 38  | 109, 160, 253, 420    | 0     |
| 38  | YS    | 111/112 (99%)  | -0.03  | 0 100 100     | 73, 102, 175, 285     | 0     |
| 39  | RT    | 137/146 (93%)  | -0.14  | 2 (1%) 73 60  | 70, 107, 263, 350     | 0     |
| 39  | YT    | 137/146 (93%)  | -0.11  | 4 (2%) 51 35  | 60, 84, 192, 451      | 0     |
| 40  | RU    | 117/118 (99%)  | 0.01   | 3 (2%) 56 40  | 62, 106, 174, 287     | 0     |
| 40  | YU    | 117/118 (99%)  | -0.27  | 1 (0%) 84 73  | 47, 71, 134, 425      | 0     |
| 41  | RV    | 101/101 (100%) | 0.27   | 7 (6%) 16 10  | 64, 129, 225, 419     | 0     |
| 41  | YV    | 101/101 (100%) | -0.08  | 2 (1%) 65 49  | 46, 89, 172, 424      | 0     |
| 42  | RW    | 113/113 (100%) | -0.11  | 3 (2%) 54 38  | 55, 75, 154, 298      | 0     |
| 42  | YW    | 113/113 (100%) | -0.15  | 1 (0%) 84 73  | 42, 67, 139, 206      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43  | RX    | 92/96 (95%)       | -0.04  | 0 100 100       | 67, 95, 161, 200      | 0     |
| 43  | YX    | 92/96 (95%)       | -0.03  | 1 (1%) 80 68    | 50, 72, 129, 260      | 0     |
| 44  | RY    | 102/110 (92%)     | 0.39   | 10 (9%) 7 4     | 79, 132, 238, 489     | 0     |
| 44  | YY    | 102/110 (92%)     | -0.04  | 3 (2%) 51 35    | 63, 103, 175, 385     | 0     |
| 45  | RZ    | 183/206 (88%)     | 0.93   | 32 (17%) 1 1    | 123, 195, 338, 497    | 0     |
| 45  | YZ    | 183/206 (88%)     | 0.63   | 23 (12%) 3 2    | 76, 148, 434, 554     | 0     |
| 46  | R0    | 82/85 (96%)       | 0.27   | 7 (8%) 10 6     | 69, 114, 152, 188     | 0     |
| 46  | Y0    | 82/85 (96%)       | -0.02  | 1 (1%) 79 66    | 47, 70, 126, 171      | 0     |
| 47  | R1    | 97/98 (98%)       | 0.34   | 3 (3%) 49 33    | 58, 95, 208, 261      | 0     |
| 47  | Y1    | 97/98 (98%)       | 0.06   | 3 (3%) 49 33    | 45, 72, 181, 340      | 0     |
| 48  | R2    | 69/72 (95%)       | -0.21  | 0 100 100       | 80, 129, 215, 245     | 0     |
| 48  | Y2    | 69/72 (95%)       | -0.06  | 0 100 100       | 60, 88, 176, 274      | 0     |
| 49  | R3    | 59/60 (98%)       | 0.22   | 3 (5%) 28 17    | 82, 121, 199, 517     | 0     |
| 49  | Y3    | 59/60 (98%)       | -0.02  | 2 (3%) 45 30    | 55, 76, 140, 319      | 0     |
| 50  | R4    | 71/71 (100%)      | 1.27   | 16 (22%) 0 0    | 132, 253, 520, 577    | 0     |
| 50  | Y4    | 71/71 (100%)      | 0.79   | 10 (14%) 2 2    | 103, 196, 455, 567    | 0     |
| 51  | R5    | 59/60 (98%)       | 0.25   | 5 (8%) 10 6     | 46, 95, 288, 394      | 0     |
| 51  | Y5    | 57/60 (95%)       | 0.11   | 1 (1%) 68 53    | 23, 73, 267, 342      | 0     |
| 52  | R6    | 49/54 (90%)       | 0.66   | 3 (6%) 21 12    | 88, 156, 225, 300     | 0     |
| 52  | Y6    | 49/54 (90%)       | 0.63   | 5 (10%) 6 4     | 53, 118, 199, 327     | 0     |
| 53  | R7    | 49/49 (100%)      | -0.26  | 0 100 100       | 38, 65, 157, 188      | 0     |
| 53  | Y7    | 49/49 (100%)      | -0.18  | 1 (2%) 65 49    | 26, 48, 108, 212      | 0     |
| 54  | R8    | 64/65 (98%)       | -0.02  | 0 100 100       | 53, 93, 152, 285      | 0     |
| 54  | Y8    | 64/65 (98%)       | -0.14  | 0 100 100       | 29, 61, 107, 272      | 0     |
| 55  | R9    | 37/37 (100%)      | 1.31   | 7 (18%) 1 0     | 92, 141, 227, 400     | 0     |
| 55  | Y9    | 37/37 (100%)      | 0.79   | 3 (8%) 12 7     | 45, 101, 162, 378     | 0     |
| 56  | Z7    | 8/12 (66%)        | 0.80   | 0 100 100       | 115, 174, 254, 280    | 0     |
| 56  | Z8    | 8/12 (66%)        | 0.43   | 0 100 100       | 124, 137, 204, 234    | 0     |
| All | All   | 21045/21776 (96%) | 0.20   | 1024 (4%) 29 18 | 23, 99, 241, 583      | 0     |

All (1024) RSRZ outliers are listed below:



| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | YE    | 205  | ALA  | 22.8 |
| 1   | QA    | 1032 | A    | 16.7 |
| 25  | RA    | 1100 | C    | 16.6 |
| 25  | RA    | 1068 | G    | 15.9 |
| 23  | XW    | 20   | U    | 14.1 |
| 25  | RA    | 1092 | C    | 13.3 |
| 25  | YA    | 1097 | U    | 13.0 |
| 25  | RA    | 1084 | A    | 13.0 |
| 25  | RA    | 1096 | A    | 12.9 |
| 45  | YZ    | 177  | PRO  | 12.8 |
| 25  | RA    | 1099 | G    | 11.3 |
| 23  | QW    | 21   | A    | 11.2 |
| 25  | RA    | 1065 | U    | 10.8 |
| 25  | YA    | 2801 | A    | 10.2 |
| 1   | QA    | 1027 | C    | 10.1 |
| 25  | RA    | 1078 | U    | 9.8  |
| 25  | RA    | 1059 | G    | 9.2  |
| 25  | RA    | 889  | C    | 9.1  |
| 25  | RA    | 1066 | U    | 9.0  |
| 45  | YZ    | 115  | GLY  | 9.0  |
| 25  | RA    | 1093 | G    | 8.9  |
| 25  | RA    | 2116 | G    | 8.9  |
| 25  | RA    | 1064 | C    | 8.8  |
| 25  | RA    | 1095 | A    | 8.2  |
| 25  | RA    | 2802 | G    | 8.2  |
| 25  | RA    | 279  | C    | 8.1  |
| 25  | RA    | 1058 | G    | 8.0  |
| 25  | RA    | 2894 | G    | 8.0  |
| 25  | RA    | 885  | C    | 7.9  |
| 25  | YA    | 2799 | A    | 7.9  |
| 25  | YA    | 1536 | A    | 7.9  |
| 1   | QA    | 1033 | G    | 7.8  |
| 25  | YA    | 1068 | G    | 7.8  |
| 1   | QA    | 1026 | G    | 7.8  |
| 25  | YA    | 884  | C    | 7.8  |
| 45  | RZ    | 114  | GLY  | 7.7  |
| 24  | QX    | 13   | A    | 7.6  |
| 25  | YA    | 2173 | A    | 7.6  |
| 1   | XA    | 1032 | A    | 7.6  |
| 45  | RZ    | 144  | LEU  | 7.6  |
| 11  | QK    | 129  | SER  | 7.6  |
| 25  | RA    | 2799 | A    | 7.5  |
| 25  | RA    | 1101 | U    | 7.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 1067 | A    | 7.3  |
| 28  | RE    | 205  | ALA  | 7.2  |
| 25  | YA    | 1096 | A    | 7.1  |
| 45  | YZ    | 113  | ALA  | 7.1  |
| 25  | RA    | 2801 | A    | 7.1  |
| 1   | QA    | 1034 | G    | 7.1  |
| 21  | QU    | 25   | LYS  | 7.1  |
| 25  | RA    | 1077 | A    | 7.0  |
| 25  | YA    | 896  | A    | 7.0  |
| 7   | QG    | 81   | GLY  | 6.9  |
| 23  | XW    | 21   | A    | 6.9  |
| 49  | R3    | 60   | GLU  | 6.8  |
| 25  | YA    | 890  | A    | 6.8  |
| 25  | RA    | 2167 | U    | 6.7  |
| 25  | YA    | 2125 | G    | 6.7  |
| 28  | YE    | 204  | ALA  | 6.7  |
| 50  | Y4    | 66   | SER  | 6.7  |
| 25  | RA    | 2173 | A    | 6.6  |
| 25  | YA    | 1098 | A    | 6.6  |
| 25  | RA    | 1063 | G    | 6.6  |
| 25  | YA    | 2167 | U    | 6.6  |
| 50  | R4    | 61   | ARG  | 6.5  |
| 25  | YA    | 2132 | U    | 6.5  |
| 23  | XW    | 17   | C    | 6.5  |
| 25  | RA    | 546  | C    | 6.4  |
| 25  | YA    | 2791 | C    | 6.4  |
| 25  | RA    | 1091 | G    | 6.3  |
| 25  | RA    | 1097 | U    | 6.3  |
| 25  | RA    | 2168 | G    | 6.3  |
| 5   | QE    | 155  | GLU  | 6.3  |
| 1   | XA    | 81   | G    | 6.3  |
| 23  | XW    | 55   | U    | 6.3  |
| 31  | RH    | 82   | GLY  | 6.2  |
| 1   | XA    | 1031 | G    | 6.2  |
| 25  | YA    | 2798 | C    | 6.2  |
| 25  | RA    | 2174 | C    | 6.2  |
| 2   | QB    | 38   | GLY  | 6.1  |
| 2   | QB    | 21   | ARG  | 6.1  |
| 45  | RZ    | 113  | ALA  | 6.0  |
| 20  | XT    | 106  | ALA  | 6.0  |
| 1   | QA    | 1531 | A    | 6.0  |
| 25  | YA    | 889  | C    | 6.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 3   | QC    | 103     | VAL  | 5.9  |
| 45  | RZ    | 107     | THR  | 5.9  |
| 25  | RA    | 2795    | G    | 5.9  |
| 11  | QK    | 128     | ALA  | 5.9  |
| 45  | RZ    | 145     | GLU  | 5.9  |
| 2   | XB    | 240     | GLN  | 5.8  |
| 7   | QG    | 82      | GLY  | 5.8  |
| 45  | YZ    | 114     | GLY  | 5.8  |
| 23  | QW    | 48      | C    | 5.8  |
| 40  | RU    | 118     | GLY  | 5.8  |
| 25  | RA    | 1088    | A    | 5.7  |
| 11  | XK    | 129     | SER  | 5.7  |
| 23  | QW    | 6       | G    | 5.7  |
| 24  | XX    | 13      | A    | 5.7  |
| 2   | XB    | 4       | GLU  | 5.7  |
| 25  | RA    | 2118    | U    | 5.7  |
| 18  | XR    | 88      | LYS  | 5.7  |
| 50  | R4    | 56      | VAL  | 5.7  |
| 1   | XA    | 344     | A    | 5.6  |
| 45  | RZ    | 177     | PRO  | 5.6  |
| 10  | QJ    | 36      | GLY  | 5.6  |
| 51  | R5    | 60      | VAL  | 5.6  |
| 25  | RA    | 887     | A    | 5.5  |
| 23  | XW    | 56      | C    | 5.4  |
| 45  | YZ    | 176     | PRO  | 5.4  |
| 25  | YA    | 2894    | G    | 5.4  |
| 25  | RA    | 890     | A    | 5.4  |
| 30  | RG    | 27      | ASN  | 5.4  |
| 3   | XC    | 194     | GLY  | 5.4  |
| 25  | YA    | 1076    | C    | 5.4  |
| 25  | RA    | 878     | A    | 5.4  |
| 25  | YA    | 2790    | A    | 5.4  |
| 45  | RZ    | 93      | ASP  | 5.4  |
| 1   | QA    | 1032(A) | G    | 5.3  |
| 25  | RA    | 1075    | C    | 5.3  |
| 23  | XW    | 61      | C    | 5.3  |
| 25  | YA    | 1084    | A    | 5.2  |
| 1   | XA    | 1451    | A    | 5.2  |
| 25  | YA    | 1058    | G    | 5.2  |
| 25  | RA    | 654     | A    | 5.2  |
| 28  | RE    | 69      | LYS  | 5.2  |
| 25  | RA    | 1094    | U    | 5.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | RA           | 2794       | C           | 5.1         |
| 40         | RU           | 117        | GLN         | 5.1         |
| 1          | QA           | 1032(B)    | G           | 5.1         |
| 25         | YA           | 277        | C           | 5.1         |
| 50         | R4           | 40         | HIS         | 5.1         |
| 23         | XW           | 16         | U           | 5.1         |
| 25         | RA           | 1098       | A           | 5.1         |
| 31         | RH           | 24         | VAL         | 5.1         |
| 1          | XA           | 1025       | U           | 5.0         |
| 2          | QB           | 19         | HIS         | 5.0         |
| 23         | QW           | 46         | G           | 5.0         |
| 45         | YZ           | 116        | VAL         | 5.0         |
| 23         | QW           | 22         | G           | 5.0         |
| 16         | XP           | 83         | GLU         | 5.0         |
| 1          | XA           | 1260       | C           | 5.0         |
| 31         | RH           | 31         | GLY         | 5.0         |
| 23         | XW           | 14         | A           | 4.9         |
| 25         | RA           | 2119       | A           | 4.9         |
| 19         | QS           | 27         | GLU         | 4.9         |
| 25         | RA           | 1053       | C           | 4.9         |
| 2          | QB           | 35         | GLU         | 4.9         |
| 44         | RY           | 52         | SER         | 4.9         |
| 25         | RA           | 1052       | C           | 4.9         |
| 23         | XW           | 24         | G           | 4.9         |
| 25         | YA           | 1057       | A           | 4.9         |
| 25         | RA           | 2113       | U           | 4.9         |
| 31         | YH           | 2          | SER         | 4.9         |
| 46         | R0           | 5          | LYS         | 4.8         |
| 35         | RP           | 118        | GLY         | 4.8         |
| 52         | R6           | 5          | VAL         | 4.8         |
| 23         | QW           | 47         | U           | 4.8         |
| 50         | Y4           | 40         | HIS         | 4.8         |
| 3          | QC           | 90         | GLU         | 4.8         |
| 1          | XA           | 1531       | A           | 4.8         |
| 25         | YA           | 2126       | A           | 4.8         |
| 23         | QW           | 45         | U           | 4.8         |
| 25         | RA           | 11         | G           | 4.7         |
| 25         | RA           | 2112       | G           | 4.7         |
| 20         | QT           | 102        | GLY         | 4.7         |
| 1          | XA           | 77         | C           | 4.7         |
| 25         | RA           | 2798       | C           | 4.7         |
| 45         | YZ           | 148        | ASP         | 4.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | XF    | 36   | ARG  | 4.7  |
| 23  | QW    | 20   | U    | 4.7  |
| 1   | QA    | 81   | G    | 4.6  |
| 1   | XA    | 1033 | G    | 4.6  |
| 2   | QB    | 240  | GLN  | 4.6  |
| 44  | YY    | 50   | ARG  | 4.6  |
| 45  | RZ    | 112  | ARG  | 4.6  |
| 25  | YA    | 899  | A    | 4.6  |
| 25  | RA    | 1074 | G    | 4.6  |
| 50  | R4    | 66   | SER  | 4.6  |
| 45  | RZ    | 108  | PRO  | 4.6  |
| 1   | QA    | 993  | G    | 4.6  |
| 25  | YA    | 2795 | G    | 4.6  |
| 25  | RA    | 1085 | A    | 4.6  |
| 25  | RA    | 2797 | U    | 4.6  |
| 1   | QA    | 88   | C    | 4.6  |
| 7   | QG    | 156  | TRP  | 4.6  |
| 23  | XW    | 23   | A    | 4.6  |
| 50  | R4    | 57   | GLU  | 4.6  |
| 25  | RA    | 645  | C    | 4.6  |
| 25  | RA    | 1061 | U    | 4.6  |
| 6   | XF    | 66   | GLU  | 4.5  |
| 23  | XW    | 35   | A    | 4.5  |
| 25  | RA    | 894  | C    | 4.5  |
| 22  | QV    | 47   | U    | 4.5  |
| 25  | RA    | 1060 | U    | 4.5  |
| 45  | YZ    | 149  | SER  | 4.5  |
| 55  | R9    | 36   | GLN  | 4.5  |
| 23  | QW    | 49   | C    | 4.5  |
| 25  | RA    | 10   | G    | 4.5  |
| 45  | YZ    | 179  | ASP  | 4.5  |
| 25  | RA    | 1107 | G    | 4.5  |
| 1   | XA    | 210  | U    | 4.5  |
| 25  | RA    | 1108 | U    | 4.5  |
| 2   | QB    | 40   | HIS  | 4.4  |
| 1   | XA    | 1161 | C    | 4.4  |
| 2   | QB    | 36   | ARG  | 4.4  |
| 50  | Y4    | 60   | GLN  | 4.4  |
| 23  | QW    | 55   | U    | 4.4  |
| 25  | RA    | 1585 | C    | 4.4  |
| 25  | RA    | 1536 | A    | 4.4  |
| 1   | QA    | 1031 | G    | 4.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 41         | RV           | 45         | THR         | 4.4         |
| 25         | RA           | 2169       | A           | 4.4         |
| 25         | YA           | 1077       | A           | 4.4         |
| 3          | QC           | 105        | GLU         | 4.4         |
| 25         | YA           | 1078       | U           | 4.3         |
| 25         | YA           | 1099       | G           | 4.3         |
| 6          | XF           | 38         | GLU         | 4.3         |
| 1          | QA           | 994        | A           | 4.3         |
| 1          | XA           | 80         | G           | 4.3         |
| 25         | YA           | 887        | A           | 4.3         |
| 49         | Y3           | 60         | GLU         | 4.3         |
| 19         | XS           | 27         | GLU         | 4.3         |
| 23         | QY           | 31         | A           | 4.3         |
| 23         | XW           | 46         | G           | 4.3         |
| 51         | Y5           | 54         | GLY         | 4.3         |
| 25         | YA           | 2116       | G           | 4.3         |
| 25         | RA           | 888        | C           | 4.3         |
| 22         | XV           | 47         | U           | 4.2         |
| 50         | R4           | 60         | GLN         | 4.2         |
| 12         | QL           | 129        | ALA         | 4.2         |
| 31         | RH           | 96         | ALA         | 4.2         |
| 25         | RA           | 884        | C           | 4.2         |
| 1          | QA           | 1029       | G           | 4.2         |
| 23         | XW           | 34         | G           | 4.2         |
| 25         | RA           | 1071       | G           | 4.2         |
| 1          | QA           | 1028       | C           | 4.2         |
| 10         | QJ           | 33         | GLN         | 4.2         |
| 12         | XL           | 129        | ALA         | 4.2         |
| 1          | XA           | 1032(A)    | G           | 4.2         |
| 2          | QB           | 37         | ASN         | 4.2         |
| 23         | XW           | 48         | C           | 4.2         |
| 25         | YA           | 893        | C           | 4.2         |
| 21         | XU           | 26         | LYS         | 4.2         |
| 25         | RA           | 2895       | U           | 4.2         |
| 9          | XI           | 95         | LYS         | 4.2         |
| 25         | RA           | 2893       | G           | 4.1         |
| 25         | YA           | 2127       | G           | 4.1         |
| 1          | XA           | 1027       | C           | 4.1         |
| 45         | RZ           | 176        | PRO         | 4.1         |
| 25         | RA           | 896        | A           | 4.1         |
| 2          | QB           | 4          | GLU         | 4.1         |
| 45         | RZ           | 115        | GLY         | 4.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | YV    | 36   | PRO  | 4.1  |
| 51  | R5    | 54   | GLY  | 4.1  |
| 25  | RA    | 1104 | C    | 4.1  |
| 23  | XW    | 47   | U    | 4.1  |
| 41  | RV    | 26   | ASP  | 4.1  |
| 1   | XA    | 1026 | G    | 4.1  |
| 25  | YA    | 654  | A    | 4.1  |
| 42  | RW    | 1    | MET  | 4.1  |
| 1   | QA    | 485  | G    | 4.0  |
| 25  | RA    | 1070 | A    | 4.0  |
| 23  | XW    | 45   | U    | 4.0  |
| 25  | RA    | 1072 | C    | 4.0  |
| 25  | RA    | 2138 | C    | 4.0  |
| 11  | QK    | 11   | LYS  | 4.0  |
| 55  | R9    | 35   | ARG  | 4.0  |
| 1   | XA    | 87   | A    | 4.0  |
| 25  | RA    | 2152 | G    | 4.0  |
| 32  | RI    | 144  | VAL  | 4.0  |
| 45  | YZ    | 173  | ALA  | 4.0  |
| 39  | YT    | 135  | ALA  | 4.0  |
| 25  | YA    | 886  | C    | 4.0  |
| 23  | XW    | 7    | A    | 4.0  |
| 31  | RH    | 33   | LEU  | 4.0  |
| 28  | RE    | 68   | ALA  | 4.0  |
| 1   | QA    | 208  | U    | 4.0  |
| 25  | YA    | 1088 | A    | 4.0  |
| 1   | XA    | 1030 | C    | 3.9  |
| 21  | QU    | 26   | LYS  | 3.9  |
| 23  | XW    | 62   | C    | 3.9  |
| 25  | YA    | 2794 | C    | 3.9  |
| 50  | R4    | 23   | GLU  | 3.9  |
| 25  | YA    | 897  | C    | 3.9  |
| 26  | RB    | 17   | C    | 3.9  |
| 25  | YA    | 2131 | G    | 3.9  |
| 25  | YA    | 898  | C    | 3.9  |
| 24  | XX    | 22   | A    | 3.8  |
| 25  | RA    | 1055 | G    | 3.8  |
| 9   | QI    | 8    | GLY  | 3.8  |
| 3   | QC    | 87   | LEU  | 3.8  |
| 3   | QC    | 104  | GLN  | 3.8  |
| 7   | XG    | 156  | TRP  | 3.8  |
| 23  | XW    | 22   | G    | 3.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 20         | QT           | 104        | LEU         | 3.8         |
| 11         | QK           | 127        | LYS         | 3.8         |
| 25         | RA           | 886        | C           | 3.8         |
| 31         | YH           | 3          | ARG         | 3.8         |
| 25         | YA           | 1075       | C           | 3.8         |
| 23         | XW           | 9          | A           | 3.8         |
| 25         | YA           | 1176       | G           | 3.8         |
| 23         | QW           | 50         | U           | 3.8         |
| 23         | QY           | 75         | C           | 3.8         |
| 25         | YA           | 878        | A           | 3.8         |
| 3          | QC           | 101        | LEU         | 3.8         |
| 1          | XA           | 76         | G           | 3.7         |
| 23         | XW           | 36         | A           | 3.7         |
| 1          | XA           | 78         | G           | 3.7         |
| 25         | YA           | 1074       | G           | 3.7         |
| 25         | RA           | 654(A)     | G           | 3.7         |
| 29         | YF           | 133        | ASN         | 3.7         |
| 16         | QP           | 84         | ALA         | 3.7         |
| 25         | RA           | 2161       | C           | 3.7         |
| 45         | RZ           | 111        | VAL         | 3.7         |
| 50         | R4           | 70         | GLY         | 3.7         |
| 2          | QB           | 5          | ILE         | 3.7         |
| 30         | RG           | 182        | LYS         | 3.7         |
| 42         | RW           | 94         | ASP         | 3.7         |
| 3          | XC           | 193        | TYR         | 3.7         |
| 31         | RH           | 137        | ASP         | 3.7         |
| 25         | RA           | 2128       | C           | 3.7         |
| 25         | YA           | 1508       | A           | 3.7         |
| 46         | R0           | 2          | ALA         | 3.7         |
| 1          | QA           | 1451       | A           | 3.7         |
| 23         | XW           | 15         | G           | 3.7         |
| 25         | RA           | 2153       | G           | 3.7         |
| 11         | XK           | 11         | LYS         | 3.6         |
| 9          | QI           | 53         | VAL         | 3.6         |
| 25         | RA           | 1102       | C           | 3.6         |
| 45         | RZ           | 92         | SER         | 3.6         |
| 1          | XA           | 1259       | C           | 3.6         |
| 45         | RZ           | 162        | GLU         | 3.6         |
| 41         | RV           | 27         | ALA         | 3.6         |
| 45         | YZ           | 112        | ARG         | 3.6         |
| 25         | RA           | 1049       | C           | 3.6         |
| 31         | RH           | 43         | VAL         | 3.6         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | RQ    | 141  | GLN  | 3.6  |
| 47  | Y1    | 97   | LEU  | 3.6  |
| 25  | RA    | 1534 | G    | 3.6  |
| 25  | YA    | 275  | G    | 3.6  |
| 25  | RA    | 1508 | A    | 3.6  |
| 45  | RZ    | 73   | GLN  | 3.6  |
| 31  | RH    | 2    | SER  | 3.6  |
| 45  | YZ    | 63   | ASP  | 3.6  |
| 9   | QI    | 95   | LYS  | 3.6  |
| 10  | QJ    | 80   | LYS  | 3.6  |
| 25  | YA    | 2166 | G    | 3.6  |
| 42  | RW    | 113  | LYS  | 3.5  |
| 25  | RA    | 1073 | A    | 3.5  |
| 25  | YA    | 276  | A    | 3.5  |
| 25  | YA    | 2797 | U    | 3.5  |
| 22  | QV    | 48   | C    | 3.5  |
| 25  | RA    | 881  | G    | 3.5  |
| 25  | RA    | 1089 | G    | 3.5  |
| 36  | RQ    | 1    | MET  | 3.5  |
| 50  | R4    | 51   | ASP  | 3.5  |
| 12  | QL    | 127  | GLU  | 3.5  |
| 25  | RA    | 1113 | U    | 3.5  |
| 2   | QB    | 39   | ILE  | 3.5  |
| 31  | RH    | 23   | ARG  | 3.5  |
| 10  | QJ    | 90   | LEU  | 3.5  |
| 13  | XM    | 120  | LYS  | 3.5  |
| 25  | RA    | 2154 | G    | 3.5  |
| 9   | QI    | 124  | GLN  | 3.5  |
| 25  | YA    | 2109 | U    | 3.5  |
| 45  | RZ    | 95   | PRO  | 3.5  |
| 25  | YA    | 883  | G    | 3.5  |
| 23  | XW    | 8    | U    | 3.5  |
| 1   | QA    | 161  | A    | 3.5  |
| 25  | RA    | 1057 | A    | 3.5  |
| 45  | RZ    | 122  | ARG  | 3.4  |
| 25  | YA    | 2141 | G    | 3.4  |
| 9   | XI    | 8    | GLY  | 3.4  |
| 39  | YT    | 129  | ARG  | 3.4  |
| 23  | QW    | 35   | A    | 3.4  |
| 25  | YA    | 2793 | G    | 3.4  |
| 32  | RI    | 86   | THR  | 3.4  |
| 25  | RA    | 2155 | G    | 3.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 44  | RY    | 89      | PHE  | 3.4  |
| 50  | Y4    | 67      | TYR  | 3.4  |
| 1   | XA    | 1032(B) | G    | 3.4  |
| 25  | YA    | 1061    | U    | 3.4  |
| 45  | RZ    | 179     | ASP  | 3.4  |
| 25  | RA    | 654(B)  | C    | 3.4  |
| 25  | YA    | 1059    | G    | 3.4  |
| 25  | RA    | 1076    | C    | 3.4  |
| 7   | XG    | 85      | TYR  | 3.4  |
| 25  | YA    | 2833    | G    | 3.3  |
| 50  | Y4    | 51      | ASP  | 3.3  |
| 25  | RA    | 1177    | A    | 3.3  |
| 1   | QA    | 1260    | C    | 3.3  |
| 2   | QB    | 112     | VAL  | 3.3  |
| 2   | QB    | 238     | LEU  | 3.3  |
| 1   | QA    | 1030    | C    | 3.3  |
| 9   | QI    | 93      | ARG  | 3.3  |
| 49  | R3    | 2       | PRO  | 3.3  |
| 23  | QW    | 34      | G    | 3.3  |
| 33  | YN    | 134     | ARG  | 3.3  |
| 3   | QC    | 68      | VAL  | 3.3  |
| 23  | QW    | 7       | A    | 3.3  |
| 25  | RA    | 2114    | A    | 3.3  |
| 25  | YA    | 546     | C    | 3.3  |
| 3   | QC    | 107     | GLN  | 3.3  |
| 25  | RA    | 882     | G    | 3.3  |
| 25  | RA    | 1087    | G    | 3.3  |
| 24  | XX    | 14      | A    | 3.3  |
| 25  | RA    | 1103    | A    | 3.3  |
| 1   | XA    | 630     | G    | 3.3  |
| 1   | XA    | 1450    | U    | 3.3  |
| 23  | XW    | 59      | U    | 3.3  |
| 50  | R4    | 62      | ARG  | 3.3  |
| 23  | XW    | 54      | U    | 3.3  |
| 25  | RA    | 879     | G    | 3.3  |
| 35  | RP    | 116     | GLY  | 3.3  |
| 25  | RA    | 1069    | A    | 3.3  |
| 7   | QG    | 85      | TYR  | 3.3  |
| 1   | XA    | 1258    | G    | 3.3  |
| 25  | RA    | 545     | G    | 3.3  |
| 25  | RA    | 2156    | G    | 3.3  |
| 45  | YZ    | 175     | VAL  | 3.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | RA           | 278        | A           | 3.2         |
| 1          | XA           | 96         | G           | 3.2         |
| 25         | RA           | 883        | G           | 3.2         |
| 5          | QE           | 154        | GLY         | 3.2         |
| 25         | YA           | 2133       | G           | 3.2         |
| 25         | YA           | 2893       | G           | 3.2         |
| 44         | RY           | 50         | ARG         | 3.2         |
| 36         | RQ           | 140        | ALA         | 3.2         |
| 22         | QV           | 20         | U           | 3.2         |
| 4          | QD           | 86         | LYS         | 3.2         |
| 10         | QJ           | 34         | VAL         | 3.2         |
| 50         | Y4           | 53         | GLU         | 3.2         |
| 50         | R4           | 6          | HIS         | 3.2         |
| 21         | QU           | 24         | ARG         | 3.2         |
| 19         | QS           | 64         | GLU         | 3.2         |
| 33         | YN           | 133        | GLN         | 3.2         |
| 25         | YA           | 2803       | C           | 3.2         |
| 25         | YA           | 1173       | G           | 3.1         |
| 1          | XA           | 345        | C           | 3.1         |
| 1          | XA           | 412        | A           | 3.1         |
| 25         | YA           | 2130       | U           | 3.1         |
| 23         | QW           | 15         | G           | 3.1         |
| 23         | XW           | 53         | G           | 3.1         |
| 28         | YE           | 41         | LYS         | 3.1         |
| 25         | RA           | 893        | C           | 3.1         |
| 25         | RA           | 2791       | C           | 3.1         |
| 26         | RB           | 16         | G           | 3.1         |
| 25         | RA           | 1082       | U           | 3.1         |
| 11         | XK           | 127        | LYS         | 3.1         |
| 25         | YA           | 654(B)     | C           | 3.1         |
| 23         | QW           | 65         | G           | 3.1         |
| 30         | RG           | 25         | TYR         | 3.1         |
| 6          | QF           | 84         | ASN         | 3.1         |
| 23         | QW           | 56         | C           | 3.1         |
| 23         | QW           | 19         | G           | 3.1         |
| 25         | RA           | 2125       | G           | 3.1         |
| 23         | QW           | 9          | A           | 3.1         |
| 32         | RI           | 16         | GLY         | 3.1         |
| 25         | YA           | 654(A)     | G           | 3.1         |
| 21         | QU           | 18         | TYR         | 3.1         |
| 25         | YA           | 1079       | C           | 3.1         |
| 52         | Y6           | 6          | ARG         | 3.1         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 25  | RA    | 2146   | C    | 3.1  |
| 10  | XJ    | 34     | VAL  | 3.1  |
| 25  | YA    | 2154   | G    | 3.1  |
| 25  | YA    | 2155   | G    | 3.1  |
| 7   | QG    | 5      | ARG  | 3.0  |
| 25  | YA    | 2892   | A    | 3.0  |
| 25  | RA    | 2833   | G    | 3.0  |
| 32  | RI    | 10     | GLU  | 3.0  |
| 39  | RT    | 137    | LYS  | 3.0  |
| 30  | RG    | 88     | ILE  | 3.0  |
| 31  | RH    | 136    | ILE  | 3.0  |
| 44  | RY    | 45     | VAL  | 3.0  |
| 1   | QA    | 1047   | G    | 3.0  |
| 1   | XA    | 631    | G    | 3.0  |
| 9   | QI    | 125    | TYR  | 3.0  |
| 28  | RE    | 204    | ALA  | 3.0  |
| 47  | R1    | 97     | LEU  | 3.0  |
| 25  | YA    | 2161   | C    | 3.0  |
| 25  | YA    | 2896   | C    | 3.0  |
| 25  | RA    | 2171   | A    | 3.0  |
| 25  | YA    | 1174   | A    | 3.0  |
| 50  | R4    | 67     | TYR  | 3.0  |
| 25  | YA    | 2164   | C    | 3.0  |
| 25  | YA    | 270(E) | G    | 3.0  |
| 40  | YU    | 117    | GLN  | 3.0  |
| 1   | QA    | 1000   | A    | 3.0  |
| 21  | XU    | 25     | LYS  | 3.0  |
| 1   | QA    | 89     | U    | 3.0  |
| 1   | QA    | 1450   | U    | 3.0  |
| 25  | RA    | 2139   | C    | 3.0  |
| 9   | XI    | 119    | ALA  | 3.0  |
| 30  | RG    | 89     | GLY  | 3.0  |
| 1   | QA    | 1009   | G    | 3.0  |
| 13  | XM    | 121    | LYS  | 3.0  |
| 15  | QO    | 89     | GLY  | 3.0  |
| 2   | XB    | 5      | ILE  | 3.0  |
| 25  | RA    | 917    | A    | 3.0  |
| 14  | QN    | 8      | GLU  | 3.0  |
| 9   | QI    | 110    | GLU  | 2.9  |
| 25  | RA    | 880    | G    | 2.9  |
| 9   | QI    | 117    | HIS  | 2.9  |
| 31  | YH    | 136    | ILE  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 1018 | C    | 2.9  |
| 41  | RV    | 64   | HIS  | 2.9  |
| 23  | QY    | 30   | G    | 2.9  |
| 31  | RH    | 34   | GLU  | 2.9  |
| 25  | RA    | 2132 | U    | 2.9  |
| 25  | RA    | 1509 | C    | 2.9  |
| 25  | YA    | 885  | C    | 2.9  |
| 4   | XD    | 45   | GLN  | 2.9  |
| 45  | RZ    | 154  | ASP  | 2.9  |
| 45  | YZ    | 144  | LEU  | 2.9  |
| 51  | R5    | 59   | GLU  | 2.9  |
| 55  | R9    | 13   | LYS  | 2.9  |
| 28  | RE    | 18   | ASP  | 2.9  |
| 1   | XA    | 1046 | A    | 2.9  |
| 25  | YA    | 547  | A    | 2.9  |
| 55  | R9    | 9    | ARG  | 2.9  |
| 42  | YW    | 113  | LYS  | 2.9  |
| 45  | YZ    | 172  | ALA  | 2.9  |
| 50  | Y4    | 39   | CYS  | 2.9  |
| 23  | QW    | 16   | U    | 2.9  |
| 25  | RA    | 362  | U    | 2.9  |
| 28  | YE    | 69   | LYS  | 2.9  |
| 5   | QE    | 6    | PHE  | 2.9  |
| 26  | RB    | 54   | G    | 2.9  |
| 1   | XA    | 1043 | C    | 2.9  |
| 2   | XB    | 6    | THR  | 2.9  |
| 3   | XC    | 100  | ALA  | 2.9  |
| 4   | XD    | 38   | TYR  | 2.9  |
| 1   | QA    | 1021 | G    | 2.9  |
| 25  | YA    | 892  | G    | 2.9  |
| 45  | RZ    | 183  | LEU  | 2.9  |
| 1   | QA    | 1278 | U    | 2.9  |
| 9   | QI    | 36   | TYR  | 2.9  |
| 29  | YF    | 134  | GLY  | 2.9  |
| 1   | QA    | 1129 | C    | 2.9  |
| 25  | YA    | 894  | C    | 2.9  |
| 44  | RY    | 55   | TYR  | 2.9  |
| 38  | RS    | 109  | GLY  | 2.8  |
| 45  | YZ    | 159  | PRO  | 2.8  |
| 1   | QA    | 842  | C    | 2.8  |
| 25  | YA    | 2168 | G    | 2.8  |
| 25  | RA    | 1111 | A    | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | RH    | 46   | GLU  | 2.8  |
| 45  | RZ    | 155  | LEU  | 2.8  |
| 18  | QR    | 54   | ARG  | 2.8  |
| 1   | QA    | 1036 | G    | 2.8  |
| 2   | XB    | 35   | GLU  | 2.8  |
| 3   | QC    | 161  | GLU  | 2.8  |
| 35  | YP    | 13   | ASN  | 2.8  |
| 28  | RE    | 1    | MET  | 2.8  |
| 18  | QR    | 20   | ALA  | 2.8  |
| 25  | RA    | 2140 | C    | 2.8  |
| 23  | QW    | 5    | G    | 2.8  |
| 25  | RA    | 1056 | G    | 2.8  |
| 25  | RA    | 2141 | G    | 2.8  |
| 25  | YA    | 1422 | G    | 2.8  |
| 36  | RQ    | 138  | ASP  | 2.8  |
| 23  | QW    | 8    | U    | 2.8  |
| 24  | XX    | 15   | A    | 2.8  |
| 25  | RA    | 1173 | G    | 2.8  |
| 41  | RV    | 28   | GLU  | 2.8  |
| 10  | XJ    | 101  | VAL  | 2.8  |
| 20  | QT    | 103  | GLY  | 2.8  |
| 23  | XW    | 13   | C    | 2.8  |
| 23  | XW    | 12   | U    | 2.8  |
| 23  | QW    | 36   | A    | 2.8  |
| 55  | R9    | 34   | GLN  | 2.8  |
| 25  | RA    | 2110 | G    | 2.8  |
| 25  | RA    | 2166 | G    | 2.8  |
| 13  | QM    | 120  | LYS  | 2.8  |
| 24  | XX    | 21   | C    | 2.8  |
| 45  | RZ    | 156  | LYS  | 2.8  |
| 29  | RF    | 133  | ASN  | 2.8  |
| 24  | QX    | 14   | A    | 2.8  |
| 46  | Y0    | 3    | HIS  | 2.7  |
| 31  | RH    | 47   | GLU  | 2.7  |
| 41  | RV    | 1    | MET  | 2.7  |
| 2   | QB    | 228  | GLY  | 2.7  |
| 39  | YT    | 136  | GLN  | 2.7  |
| 25  | YA    | 880  | G    | 2.7  |
| 1   | XA    | 1129 | C    | 2.7  |
| 25  | YA    | 2175 | C    | 2.7  |
| 36  | YQ    | 141  | GLN  | 2.7  |
| 25  | RA    | 229  | A    | 2.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 47         | R1           | 98         | LEU         | 2.7         |
| 1          | QA           | 210        | U           | 2.7         |
| 10         | QJ           | 4          | ILE         | 2.7         |
| 23         | QW           | 54         | U           | 2.7         |
| 32         | YI           | 107        | VAL         | 2.7         |
| 23         | XW           | 6          | G           | 2.7         |
| 25         | YA           | 1063       | G           | 2.7         |
| 25         | YA           | 2802       | G           | 2.7         |
| 26         | RB           | 56         | G           | 2.7         |
| 25         | YA           | 2119       | A           | 2.7         |
| 47         | Y1           | 96         | LYS         | 2.7         |
| 14         | QN           | 61         | TRP         | 2.7         |
| 9          | XI           | 110        | GLU         | 2.7         |
| 23         | XW           | 52         | G           | 2.7         |
| 25         | YA           | 888        | C           | 2.7         |
| 51         | R5           | 52         | TYR         | 2.7         |
| 2          | QB           | 116        | GLU         | 2.7         |
| 25         | RA           | 1083       | U           | 2.7         |
| 25         | YA           | 1060       | U           | 2.7         |
| 10         | XJ           | 36         | GLY         | 2.7         |
| 19         | QS           | 85         | LYS         | 2.7         |
| 25         | RA           | 6          | A           | 2.7         |
| 45         | YZ           | 104        | PHE         | 2.7         |
| 2          | XB           | 96         | ARG         | 2.7         |
| 2          | QB           | 79         | ASP         | 2.7         |
| 12         | XL           | 128        | ALA         | 2.7         |
| 25         | RA           | 2175       | C           | 2.7         |
| 25         | YA           | 1093       | G           | 2.7         |
| 26         | RB           | 53         | A           | 2.7         |
| 2          | XB           | 229        | VAL         | 2.7         |
| 1          | QA           | 1025       | U           | 2.7         |
| 1          | XA           | 79         | G           | 2.7         |
| 23         | QW           | 53         | G           | 2.7         |
| 30         | YG           | 89         | GLY         | 2.7         |
| 1          | QA           | 1113       | C           | 2.7         |
| 44         | YY           | 52         | SER         | 2.7         |
| 45         | YZ           | 178        | GLU         | 2.7         |
| 25         | RA           | 1112       | G           | 2.7         |
| 1          | QA           | 1046       | A           | 2.6         |
| 3          | QC           | 147        | LYS         | 2.6         |
| 25         | RA           | 2793       | G           | 2.6         |
| 25         | YA           | 1421       | G           | 2.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | YA           | 2162       | G           | 2.6         |
| 28         | YE           | 68         | ALA         | 2.6         |
| 45         | RZ           | 143        | GLY         | 2.6         |
| 1          | XA           | 999        | U           | 2.6         |
| 25         | RA           | 2896       | C           | 2.6         |
| 7          | QG           | 4          | ARG         | 2.6         |
| 10         | XJ           | 71         | LEU         | 2.6         |
| 25         | RA           | 1586       | A           | 2.6         |
| 31         | RH           | 35         | VAL         | 2.6         |
| 25         | YA           | 362        | U           | 2.6         |
| 45         | YZ           | 174        | VAL         | 2.6         |
| 25         | RA           | 897        | C           | 2.6         |
| 25         | YA           | 1095       | A           | 2.6         |
| 25         | YA           | 2629       | A           | 2.6         |
| 10         | XJ           | 73         | ASP         | 2.6         |
| 1          | QA           | 1024       | G           | 2.6         |
| 3          | QC           | 59         | ARG         | 2.6         |
| 23         | QY           | 28         | G           | 2.6         |
| 23         | QY           | 29         | G           | 2.6         |
| 25         | RA           | 2151       | G           | 2.6         |
| 2          | XB           | 37         | ASN         | 2.6         |
| 25         | RA           | 1914       | C           | 2.6         |
| 2          | QB           | 231        | GLU         | 2.6         |
| 2          | QB           | 234        | PRO         | 2.6         |
| 1          | XA           | 92         | G           | 2.6         |
| 1          | XA           | 993        | G           | 2.6         |
| 5          | QE           | 5          | ASP         | 2.6         |
| 23         | QW           | 24         | G           | 2.6         |
| 25         | YA           | 1100       | C           | 2.6         |
| 25         | RA           | 2630       | G           | 2.6         |
| 32         | RI           | 60         | GLU         | 2.6         |
| 9          | QI           | 126        | SER         | 2.6         |
| 2          | QB           | 113        | HIS         | 2.6         |
| 10         | XJ           | 37         | PRO         | 2.6         |
| 1          | XA           | 73         | G           | 2.6         |
| 3          | QC           | 162        | GLN         | 2.6         |
| 25         | RA           | 1062       | G           | 2.6         |
| 25         | RA           | 1545       | A           | 2.6         |
| 45         | RZ           | 159        | PRO         | 2.6         |
| 1          | XA           | 91         | C           | 2.6         |
| 9          | QI           | 94         | ALA         | 2.6         |
| 55         | R9           | 1          | MET         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 23         | QW           | 59         | U           | 2.5         |
| 1          | QA           | 1323       | G           | 2.5         |
| 25         | RA           | 1176       | G           | 2.5         |
| 47         | Y1           | 98         | LEU         | 2.5         |
| 44         | RY           | 103        | GLY         | 2.5         |
| 9          | QI           | 116        | LYS         | 2.5         |
| 1          | QA           | 856        | C           | 2.5         |
| 10         | XJ           | 61         | GLU         | 2.5         |
| 31         | RH           | 36         | PRO         | 2.5         |
| 7          | QG           | 86         | GLN         | 2.5         |
| 7          | XG           | 78         | ARG         | 2.5         |
| 36         | RQ           | 33         | GLY         | 2.5         |
| 1          | QA           | 1087       | G           | 2.5         |
| 25         | RA           | 892        | G           | 2.5         |
| 10         | QJ           | 59         | SER         | 2.5         |
| 35         | RP           | 94         | GLU         | 2.5         |
| 23         | QW           | 64         | A           | 2.5         |
| 5          | QE           | 24         | ARG         | 2.5         |
| 25         | RA           | 88         | G           | 2.5         |
| 25         | YA           | 2110       | G           | 2.5         |
| 12         | XL           | 127        | GLU         | 2.5         |
| 52         | Y6           | 5          | VAL         | 2.5         |
| 46         | R0           | 4          | LYS         | 2.5         |
| 46         | R0           | 8          | GLY         | 2.5         |
| 15         | QO           | 28         | GLN         | 2.5         |
| 25         | RA           | 899        | A           | 2.5         |
| 25         | RA           | 2137       | C           | 2.5         |
| 33         | RN           | 9          | VAL         | 2.5         |
| 36         | YQ           | 138        | ASP         | 2.5         |
| 52         | Y6           | 26         | ASN         | 2.5         |
| 3          | QC           | 155        | GLY         | 2.5         |
| 25         | YA           | 2112       | G           | 2.5         |
| 25         | RA           | 895        | U           | 2.5         |
| 1          | QA           | 1035       | A           | 2.5         |
| 1          | XA           | 1137       | C           | 2.5         |
| 25         | RA           | 1054       | A           | 2.5         |
| 25         | YA           | 270(D)     | C           | 2.5         |
| 47         | R1           | 55         | GLY         | 2.5         |
| 18         | QR           | 88         | LYS         | 2.5         |
| 5          | XE           | 154        | GLY         | 2.5         |
| 25         | RA           | 214        | G           | 2.5         |
| 25         | YA           | 1062       | G           | 2.5         |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | RI    | 123     | LEU  | 2.5  |
| 33  | RN    | 134     | ARG  | 2.5  |
| 25  | YA    | 1507    | A    | 2.5  |
| 2   | QB    | 193     | ASP  | 2.5  |
| 32  | YI    | 65      | ALA  | 2.5  |
| 1   | XA    | 1212    | U    | 2.5  |
| 44  | RY    | 56      | PRO  | 2.5  |
| 19  | XS    | 85      | LYS  | 2.5  |
| 1   | XA    | 1131    | G    | 2.5  |
| 1   | QA    | 1236    | A    | 2.5  |
| 3   | XC    | 15      | THR  | 2.5  |
| 23  | QW    | 13      | C    | 2.5  |
| 25  | RA    | 654(T)  | C    | 2.5  |
| 19  | XS    | 84      | GLY  | 2.5  |
| 25  | RA    | 1026    | U    | 2.5  |
| 45  | RZ    | 163     | LEU  | 2.5  |
| 46  | R0    | 7       | LEU  | 2.5  |
| 25  | RA    | 270(O)  | U    | 2.5  |
| 2   | QB    | 233     | SER  | 2.4  |
| 23  | QY    | 74      | C    | 2.4  |
| 25  | RA    | 1121    | C    | 2.4  |
| 45  | RZ    | 116     | VAL  | 2.4  |
| 35  | RP    | 105     | LEU  | 2.4  |
| 3   | XC    | 88      | ARG  | 2.4  |
| 3   | XC    | 99      | VAL  | 2.4  |
| 11  | XK    | 12      | ARG  | 2.4  |
| 1   | QA    | 1045    | C    | 2.4  |
| 23  | QW    | 63      | G    | 2.4  |
| 2   | QB    | 229     | VAL  | 2.4  |
| 30  | YG    | 79      | ASN  | 2.4  |
| 35  | RP    | 120     | ALA  | 2.4  |
| 10  | QJ    | 74      | ILE  | 2.4  |
| 30  | RG    | 52      | ILE  | 2.4  |
| 1   | QA    | 162     | A    | 2.4  |
| 9   | XI    | 106     | ALA  | 2.4  |
| 1   | XA    | 998     | G    | 2.4  |
| 25  | RA    | 1114    | G    | 2.4  |
| 25  | RA    | 1545(A) | A    | 2.4  |
| 25  | RA    | 2170    | A    | 2.4  |
| 26  | RB    | 31      | C    | 2.4  |
| 28  | RE    | 200     | GLU  | 2.4  |
| 2   | QB    | 125     | PRO  | 2.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 30  | RG    | 26      | GLN  | 2.4  |
| 52  | R6    | 6       | ARG  | 2.4  |
| 22  | QV    | 21      | A    | 2.4  |
| 25  | RA    | 273(F)  | C    | 2.4  |
| 25  | RA    | 2111    | C    | 2.4  |
| 25  | YA    | 2156    | G    | 2.4  |
| 26  | RB    | 117     | G    | 2.4  |
| 27  | RD    | 2       | ALA  | 2.4  |
| 6   | XF    | 55      | ASP  | 2.4  |
| 38  | RS    | 83      | LYS  | 2.4  |
| 3   | XC    | 76      | VAL  | 2.4  |
| 10  | XJ    | 6       | ILE  | 2.4  |
| 25  | YA    | 2117    | A    | 2.4  |
| 39  | YT    | 112     | ARG  | 2.4  |
| 51  | R5    | 55      | ARG  | 2.4  |
| 35  | RP    | 1       | MET  | 2.4  |
| 1   | XA    | 1034    | G    | 2.4  |
| 25  | RA    | 2133    | G    | 2.4  |
| 25  | YA    | 2157    | G    | 2.4  |
| 31  | RH    | 32      | GLU  | 2.4  |
| 36  | RQ    | 32      | TYR  | 2.4  |
| 16  | XP    | 62      | VAL  | 2.4  |
| 23  | QW    | 62      | C    | 2.4  |
| 25  | YA    | 229     | A    | 2.4  |
| 32  | RI    | 85      | GLU  | 2.4  |
| 25  | RA    | 2100    | G    | 2.4  |
| 25  | YA    | 1888    | G    | 2.4  |
| 45  | YZ    | 147     | GLY  | 2.4  |
| 52  | Y6    | 29      | ASN  | 2.4  |
| 1   | QA    | 1303    | C    | 2.4  |
| 1   | XA    | 1028(B) | C    | 2.4  |
| 4   | XD    | 44      | GLY  | 2.4  |
| 25  | RA    | 1505    | C    | 2.4  |
| 3   | QC    | 98      | ASN  | 2.4  |
| 50  | R4    | 20      | ASN  | 2.4  |
| 50  | R4    | 22      | ILE  | 2.4  |
| 1   | XA    | 856     | C    | 2.4  |
| 25  | RA    | 918     | A    | 2.4  |
| 25  | RA    | 2803    | C    | 2.4  |
| 25  | RA    | 274     | G    | 2.4  |
| 25  | YA    | 2165    | G    | 2.4  |
| 25  | YA    | 2792    | G    | 2.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 29         | YF           | 8          | GLN         | 2.4         |
| 11         | QK           | 118        | GLY         | 2.4         |
| 25         | RA           | 2629       | A           | 2.4         |
| 26         | RB           | 78         | A           | 2.4         |
| 22         | XV           | 48         | C           | 2.4         |
| 25         | YA           | 645        | C           | 2.4         |
| 25         | YA           | 1532       | C           | 2.4         |
| 44         | YY           | 99         | CYS         | 2.3         |
| 31         | RH           | 95         | ARG         | 2.3         |
| 45         | YZ           | 107        | THR         | 2.3         |
| 15         | QO           | 15         | PHE         | 2.3         |
| 25         | RA           | 654(S)     | G           | 2.3         |
| 25         | RA           | 2160       | G           | 2.3         |
| 5          | XE           | 155        | GLU         | 2.3         |
| 23         | QW           | 11         | C           | 2.3         |
| 25         | RA           | 1079       | C           | 2.3         |
| 28         | RE           | 158        | GLY         | 2.3         |
| 9          | XI           | 94         | ALA         | 2.3         |
| 37         | RR           | 59         | ASP         | 2.3         |
| 1          | QA           | 1086       | U           | 2.3         |
| 25         | RA           | 270(M)     | U           | 2.3         |
| 26         | RB           | 29         | A           | 2.3         |
| 25         | YA           | 2140       | C           | 2.3         |
| 35         | RP           | 117        | GLU         | 2.3         |
| 29         | YF           | 16         | GLY         | 2.3         |
| 10         | QJ           | 58         | ASP         | 2.3         |
| 30         | RG           | 40         | ASN         | 2.3         |
| 50         | Y4           | 1          | MET         | 2.3         |
| 1          | QA           | 1156       | G           | 2.3         |
| 50         | R4           | 49         | PHE         | 2.3         |
| 31         | RH           | 83         | TYR         | 2.3         |
| 55         | Y9           | 30         | PRO         | 2.3         |
| 9          | XI           | 105        | ASP         | 2.3         |
| 3          | XC           | 101        | LEU         | 2.3         |
| 6          | QF           | 39         | LYS         | 2.3         |
| 25         | RA           | 2411       | A           | 2.3         |
| 25         | RA           | 1017       | G           | 2.3         |
| 26         | RB           | 55         | U           | 2.3         |
| 31         | YH           | 59         | ARG         | 2.3         |
| 45         | RZ           | 23         | LYS         | 2.3         |
| 23         | XW           | 67         | C           | 2.3         |
| 3          | QC           | 89         | GLU         | 2.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | XJ    | 4    | ILE  | 2.3  |
| 7   | QG    | 74   | GLU  | 2.3  |
| 10  | QJ    | 91   | PRO  | 2.3  |
| 49  | Y3    | 59   | VAL  | 2.3  |
| 7   | QG    | 6    | ARG  | 2.2  |
| 10  | QJ    | 83   | GLU  | 2.2  |
| 5   | QE    | 19   | MET  | 2.2  |
| 14  | QN    | 38   | GLY  | 2.2  |
| 41  | YV    | 26   | ASP  | 2.2  |
| 3   | QC    | 50   | ALA  | 2.2  |
| 17  | XQ    | 79   | SER  | 2.2  |
| 22  | XV    | 20   | U    | 2.2  |
| 25  | RA    | 1478 | G    | 2.2  |
| 25  | RA    | 2104 | G    | 2.2  |
| 25  | YA    | 2151 | G    | 2.2  |
| 41  | RV    | 17   | GLY  | 2.2  |
| 28  | YE    | 37   | ARG  | 2.2  |
| 32  | RI    | 7    | GLU  | 2.2  |
| 31  | RH    | 4    | ILE  | 2.2  |
| 25  | RA    | 2349 | G    | 2.2  |
| 25  | YA    | 2124 | G    | 2.2  |
| 26  | RB    | 102  | G    | 2.2  |
| 35  | RP    | 119  | GLU  | 2.2  |
| 3   | QC    | 194  | GLY  | 2.2  |
| 31  | RH    | 25   | LYS  | 2.2  |
| 2   | XB    | 228  | GLY  | 2.2  |
| 44  | RY    | 58   | GLY  | 2.2  |
| 45  | RZ    | 96   | VAL  | 2.2  |
| 46  | R0    | 61   | ALA  | 2.2  |
| 46  | R0    | 3    | HIS  | 2.2  |
| 25  | RA    | 1299 | G    | 2.2  |
| 1   | QA    | 82   | U    | 2.2  |
| 31  | RH    | 75   | ALA  | 2.2  |
| 2   | XB    | 40   | HIS  | 2.2  |
| 10  | QJ    | 5    | ARG  | 2.2  |
| 23  | XW    | 19   | G    | 2.2  |
| 26  | YB    | 87   | G    | 2.2  |
| 1   | QA    | 1269 | A    | 2.2  |
| 31  | RH    | 39   | PRO  | 2.2  |
| 29  | RF    | 134  | GLY  | 2.2  |
| 32  | YI    | 66   | GLU  | 2.2  |
| 9   | QI    | 7    | THR  | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 32         | RI           | 57         | ARG         | 2.2         |
| 24         | QX           | 15         | A           | 2.2         |
| 25         | RA           | 861        | A           | 2.2         |
| 25         | RA           | 1726       | G           | 2.2         |
| 3          | QC           | 86         | VAL         | 2.2         |
| 55         | Y9           | 1          | MET         | 2.2         |
| 1          | QA           | 1122       | U           | 2.2         |
| 25         | YA           | 1066       | U           | 2.2         |
| 30         | RG           | 2          | PRO         | 2.2         |
| 45         | RZ           | 55         | HIS         | 2.2         |
| 22         | QV           | 46         | G           | 2.2         |
| 25         | YA           | 1171       | G           | 2.2         |
| 1          | QA           | 1008       | C           | 2.2         |
| 1          | XA           | 1257       | U           | 2.2         |
| 2          | QB           | 230        | VAL         | 2.2         |
| 3          | QC           | 72         | LYS         | 2.2         |
| 50         | Y4           | 61         | ARG         | 2.2         |
| 23         | XY           | 41         | C           | 2.2         |
| 26         | RB           | 18         | G           | 2.2         |
| 20         | QT           | 9          | ASN         | 2.2         |
| 11         | QK           | 12         | ARG         | 2.2         |
| 21         | QU           | 22         | ARG         | 2.2         |
| 43         | YX           | 66         | LEU         | 2.2         |
| 49         | R3           | 58         | VAL         | 2.2         |
| 23         | QY           | 32         | U           | 2.2         |
| 11         | QK           | 41         | THR         | 2.1         |
| 44         | RY           | 47         | LYS         | 2.1         |
| 23         | QY           | 41         | C           | 2.1         |
| 25         | YA           | 270(N)     | G           | 2.1         |
| 31         | RH           | 135        | GLY         | 2.1         |
| 37         | YR           | 1          | MET         | 2.1         |
| 9          | XI           | 128        | ARG         | 2.1         |
| 39         | RT           | 125        | ARG         | 2.1         |
| 33         | RN           | 8          | GLN         | 2.1         |
| 25         | RA           | 1510       | A           | 2.1         |
| 1          | QA           | 570        | G           | 2.1         |
| 25         | YA           | 281        | G           | 2.1         |
| 7          | XG           | 4          | ARG         | 2.1         |
| 25         | YA           | 1070       | A           | 2.1         |
| 1          | XA           | 998(A)     | C           | 2.1         |
| 36         | YQ           | 60         | ARG         | 2.1         |
| 25         | YA           | 270(O)     | U           | 2.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | YA           | 877        | U           | 2.1         |
| 1          | QA           | 855        | G           | 2.1         |
| 7          | XG           | 52         | GLU         | 2.1         |
| 25         | YA           | 1534       | G           | 2.1         |
| 25         | YA           | 2123       | G           | 2.1         |
| 12         | QL           | 128        | ALA         | 2.1         |
| 30         | RG           | 76         | SER         | 2.1         |
| 30         | RG           | 97         | ASP         | 2.1         |
| 19         | XS           | 28         | LYS         | 2.1         |
| 25         | YA           | 1178       | C           | 2.1         |
| 25         | YA           | 1585       | C           | 2.1         |
| 26         | RB           | 27         | C           | 2.1         |
| 45         | RZ           | 110        | GLY         | 2.1         |
| 2          | XB           | 36         | ARG         | 2.1         |
| 50         | Y4           | 50         | VAL         | 2.1         |
| 32         | RI           | 8          | PRO         | 2.1         |
| 2          | XB           | 156        | LYS         | 2.1         |
| 2          | QB           | 23         | ARG         | 2.1         |
| 4          | QD           | 42         | GLN         | 2.1         |
| 25         | RA           | 1048       | A           | 2.1         |
| 25         | YA           | 2171       | A           | 2.1         |
| 31         | YH           | 72         | ILE         | 2.1         |
| 23         | XW           | 11         | C           | 2.1         |
| 36         | RQ           | 139        | GLU         | 2.1         |
| 3          | QC           | 91         | LEU         | 2.1         |
| 30         | RG           | 28         | VAL         | 2.1         |
| 50         | R4           | 50         | VAL         | 2.1         |
| 52         | Y6           | 37         | ARG         | 2.1         |
| 6          | XF           | 57         | GLN         | 2.1         |
| 19         | QS           | 10         | PHE         | 2.1         |
| 1          | QA           | 79         | G           | 2.1         |
| 25         | YA           | 654(S)     | G           | 2.1         |
| 55         | R9           | 24         | TYR         | 2.1         |
| 16         | QP           | 48         | TRP         | 2.1         |
| 25         | RA           | 363(A)     | A           | 2.1         |
| 32         | YI           | 117        | GLU         | 2.1         |
| 38         | RS           | 9          | ARG         | 2.1         |
| 30         | RG           | 53         | LEU         | 2.1         |
| 1          | XA           | 221        | C           | 2.1         |
| 9          | XI           | 127        | LYS         | 2.1         |
| 25         | RA           | 280        | C           | 2.1         |
| 25         | YA           | 2129       | C           | 2.1         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | XB    | 21     | ARG  | 2.1  |
| 45  | YZ    | 117    | LEU  | 2.1  |
| 25  | RA    | 175    | G    | 2.1  |
| 25  | YA    | 2153   | G    | 2.1  |
| 53  | Y7    | 48     | LYS  | 2.1  |
| 25  | RA    | 654(U) | A    | 2.1  |
| 1   | XA    | 1160   | G    | 2.1  |
| 25  | RA    | 653    | A    | 2.1  |
| 25  | RA    | 1122   | G    | 2.1  |
| 27  | YD    | 26     | LYS  | 2.1  |
| 23  | QW    | 66     | U    | 2.1  |
| 1   | QA    | 196    | A    | 2.0  |
| 45  | RZ    | 2      | GLU  | 2.1  |
| 44  | RY    | 87     | LYS  | 2.0  |
| 1   | QA    | 1001   | G    | 2.0  |
| 25  | RA    | 1042   | G    | 2.0  |
| 25  | RA    | 1448   | G    | 2.0  |
| 2   | QB    | 33     | TYR  | 2.0  |
| 10  | XJ    | 100    | THR  | 2.0  |
| 13  | QM    | 3      | ARG  | 2.0  |
| 1   | QA    | 1256   | A    | 2.0  |
| 22  | QV    | 59     | A    | 2.0  |
| 1   | QA    | 466    | C    | 2.0  |
| 1   | QA    | 1270   | C    | 2.0  |
| 1   | XA    | 442    | C    | 2.0  |
| 23  | QY    | 40     | C    | 2.0  |
| 26  | RB    | 79     | C    | 2.0  |
| 52  | R6    | 46     | HIS  | 2.0  |
| 9   | QI    | 54     | ASP  | 2.0  |
| 3   | QC    | 96     | GLY  | 2.0  |
| 25  | YA    | 2897   | U    | 2.0  |
| 3   | QC    | 102    | ASN  | 2.0  |
| 12  | XL    | 15     | ARG  | 2.0  |
| 30  | RG    | 50     | ALA  | 2.0  |
| 1   | QA    | 1271   | G    | 2.0  |
| 40  | RU    | 91     | ASP  | 2.0  |
| 22  | XV    | 16     | C    | 2.0  |
| 25  | RA    | 1109   | C    | 2.0  |
| 25  | RA    | 1638   | C    | 2.0  |
| 20  | XT    | 9      | ASN  | 2.0  |
| 45  | RZ    | 146    | ILE  | 2.0  |
| 45  | YZ    | 21     | ALA  | 2.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 3   | XC    | 196     | LEU  | 2.0  |
| 30  | RG    | 80      | PHE  | 2.0  |
| 1   | QA    | 478     | A    | 2.0  |
| 10  | QJ    | 73      | ASP  | 2.0  |
| 25  | RA    | 1637    | A    | 2.0  |
| 19  | XS    | 2       | PRO  | 2.0  |
| 1   | QA    | 1028(A) | C    | 2.0  |
| 25  | RA    | 2164    | C    | 2.0  |
| 55  | Y9    | 32      | HIS  | 2.0  |
| 9   | QI    | 91      | ASP  | 2.0  |
| 15  | XO    | 21      | ASP  | 2.0  |
| 7   | QG    | 80      | VAL  | 2.0  |
| 31  | RH    | 138     | LYS  | 2.0  |
| 23  | QW    | 14      | A    | 2.0  |
| 30  | RG    | 72      | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 57  | MG   | RA    | 3206 | 1/1   | -0.03 | 0.75 | 140,140,140,140            | 0     |
| 57  | MG   | RA    | 3201 | 1/1   | 0.08  | 1.74 | 128,128,128,128            | 0     |
| 57  | MG   | RA    | 3215 | 1/1   | 0.09  | 0.35 | 68,68,68,68                | 0     |
| 57  | MG   | RA    | 3225 | 1/1   | 0.19  | 0.67 | 161,161,161,161            | 0     |
| 57  | MG   | R0    | 101  | 1/1   | 0.29  | 0.61 | 78,78,78,78                | 0     |
| 57  | MG   | RA    | 3219 | 1/1   | 0.30  | 0.78 | 138,138,138,138            | 0     |
| 57  | MG   | RA    | 3217 | 1/1   | 0.33  | 0.66 | 133,133,133,133            | 0     |
| 57  | MG   | RD    | 301  | 1/1   | 0.34  | 1.06 | 91,91,91,91                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3178 | 1/1   | 0.37 | 0.50 | 64,64,64,64                 | 0     |
| 57  | MG   | XA    | 1662 | 1/1   | 0.38 | 0.71 | 61,61,61,61                 | 0     |
| 57  | MG   | XA    | 1650 | 1/1   | 0.39 | 0.68 | 60,60,60,60                 | 0     |
| 57  | MG   | RA    | 3152 | 1/1   | 0.40 | 0.30 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3224 | 1/1   | 0.41 | 0.61 | 91,91,91,91                 | 0     |
| 57  | MG   | QA    | 1649 | 1/1   | 0.41 | 0.62 | 104,104,104,104             | 0     |
| 57  | MG   | QA    | 1664 | 1/1   | 0.42 | 0.52 | 78,78,78,78                 | 0     |
| 57  | MG   | RA    | 3220 | 1/1   | 0.42 | 0.60 | 83,83,83,83                 | 0     |
| 57  | MG   | RA    | 3161 | 1/1   | 0.45 | 1.15 | 76,76,76,76                 | 0     |
| 57  | MG   | QA    | 1644 | 1/1   | 0.46 | 0.50 | 114,114,114,114             | 0     |
| 57  | MG   | RA    | 3218 | 1/1   | 0.46 | 1.01 | 132,132,132,132             | 0     |
| 57  | MG   | YA    | 3149 | 1/1   | 0.47 | 1.62 | 106,106,106,106             | 0     |
| 57  | MG   | QA    | 1633 | 1/1   | 0.47 | 0.16 | 143,143,143,143             | 0     |
| 57  | MG   | YA    | 3169 | 1/1   | 0.48 | 0.28 | 93,93,93,93                 | 0     |
| 57  | MG   | RA    | 3164 | 1/1   | 0.48 | 0.75 | 82,82,82,82                 | 0     |
| 57  | MG   | YA    | 3155 | 1/1   | 0.49 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3229 | 1/1   | 0.51 | 0.35 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3153 | 1/1   | 0.53 | 0.78 | 63,63,63,63                 | 0     |
| 57  | MG   | XA    | 1634 | 1/1   | 0.53 | 0.54 | 98,98,98,98                 | 0     |
| 57  | MG   | QA    | 1603 | 1/1   | 0.55 | 2.24 | 66,66,66,66                 | 0     |
| 57  | MG   | RA    | 3159 | 1/1   | 0.57 | 0.75 | 72,72,72,72                 | 0     |
| 57  | MG   | RA    | 3216 | 1/1   | 0.58 | 0.70 | 110,110,110,110             | 0     |
| 57  | MG   | XA    | 1666 | 1/1   | 0.58 | 0.30 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3165 | 1/1   | 0.59 | 0.34 | 77,77,77,77                 | 0     |
| 57  | MG   | YA    | 3141 | 1/1   | 0.60 | 0.39 | 69,69,69,69                 | 0     |
| 57  | MG   | QA    | 1632 | 1/1   | 0.60 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | YA    | 3224 | 1/1   | 0.61 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3254 | 1/1   | 0.61 | 0.65 | 61,61,61,61                 | 0     |
| 57  | MG   | QH    | 201  | 1/1   | 0.61 | 0.38 | 105,105,105,105             | 0     |
| 57  | MG   | RA    | 3002 | 1/1   | 0.61 | 1.24 | 70,70,70,70                 | 0     |
| 57  | MG   | YA    | 3274 | 1/1   | 0.62 | 0.61 | 57,57,57,57                 | 0     |
| 57  | MG   | RA    | 3127 | 1/1   | 0.62 | 0.45 | 74,74,74,74                 | 0     |
| 57  | MG   | RA    | 3196 | 1/1   | 0.62 | 0.41 | 108,108,108,108             | 0     |
| 57  | MG   | RA    | 3007 | 1/1   | 0.62 | 0.55 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3156 | 1/1   | 0.63 | 0.22 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3158 | 1/1   | 0.64 | 0.34 | 69,69,69,69                 | 0     |
| 57  | MG   | RA    | 3157 | 1/1   | 0.65 | 0.53 | 54,54,54,54                 | 0     |
| 57  | MG   | RA    | 3139 | 1/1   | 0.65 | 0.27 | 70,70,70,70                 | 0     |
| 57  | MG   | RA    | 3138 | 1/1   | 0.65 | 1.69 | 95,95,95,95                 | 0     |
| 57  | MG   | YA    | 3201 | 1/1   | 0.65 | 0.42 | 61,61,61,61                 | 0     |
| 57  | MG   | XA    | 1601 | 1/1   | 0.66 | 0.66 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | QA    | 1655 | 1/1   | 0.67 | 0.62 | 74,74,74,74                 | 0     |
| 57  | MG   | RA    | 3136 | 1/1   | 0.68 | 0.39 | 105,105,105,105             | 0     |
| 57  | MG   | YA    | 3156 | 1/1   | 0.68 | 0.40 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3118 | 1/1   | 0.69 | 0.63 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3243 | 1/1   | 0.69 | 0.44 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3210 | 1/1   | 0.69 | 0.43 | 135,135,135,135             | 0     |
| 57  | MG   | YA    | 3259 | 1/1   | 0.69 | 0.62 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3044 | 1/1   | 0.69 | 1.29 | 75,75,75,75                 | 0     |
| 57  | MG   | RA    | 3213 | 1/1   | 0.70 | 0.25 | 62,62,62,62                 | 0     |
| 57  | MG   | YB    | 201  | 1/1   | 0.70 | 0.45 | 57,57,57,57                 | 0     |
| 57  | MG   | RA    | 3212 | 1/1   | 0.71 | 0.54 | 89,89,89,89                 | 0     |
| 57  | MG   | YA    | 3179 | 1/1   | 0.71 | 0.29 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3175 | 1/1   | 0.71 | 0.96 | 57,57,57,57                 | 0     |
| 57  | MG   | XA    | 1628 | 1/1   | 0.71 | 0.25 | 41,41,41,41                 | 0     |
| 57  | MG   | QA    | 1629 | 1/1   | 0.71 | 0.35 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3153 | 1/1   | 0.72 | 0.46 | 79,79,79,79                 | 0     |
| 57  | MG   | XA    | 1664 | 1/1   | 0.72 | 0.25 | 51,51,51,51                 | 0     |
| 57  | MG   | XA    | 1608 | 1/1   | 0.72 | 0.69 | 119,119,119,119             | 0     |
| 57  | MG   | XA    | 1607 | 1/1   | 0.73 | 0.24 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3132 | 1/1   | 0.73 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | QA    | 1626 | 1/1   | 0.73 | 0.22 | 156,156,156,156             | 0     |
| 57  | MG   | XA    | 1670 | 1/1   | 0.73 | 0.45 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3228 | 1/1   | 0.73 | 0.67 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3233 | 1/1   | 0.73 | 0.60 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3151 | 1/1   | 0.73 | 0.26 | 69,69,69,69                 | 0     |
| 57  | MG   | RP    | 204  | 1/1   | 0.74 | 0.42 | 183,183,183,183             | 0     |
| 57  | MG   | XA    | 1651 | 1/1   | 0.74 | 0.39 | 111,111,111,111             | 0     |
| 57  | MG   | QA    | 1639 | 1/1   | 0.74 | 0.32 | 49,49,49,49                 | 0     |
| 57  | MG   | XA    | 1653 | 1/1   | 0.74 | 0.33 | 83,83,83,83                 | 0     |
| 57  | MG   | YA    | 3012 | 1/1   | 0.75 | 0.97 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3258 | 1/1   | 0.75 | 1.08 | 68,68,68,68                 | 0     |
| 57  | MG   | YA    | 3161 | 1/1   | 0.75 | 0.58 | 43,43,43,43                 | 0     |
| 57  | MG   | QA    | 1651 | 1/1   | 0.75 | 0.31 | 49,49,49,49                 | 0     |
| 57  | MG   | QA    | 1638 | 1/1   | 0.75 | 0.45 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3239 | 1/1   | 0.76 | 0.95 | 90,90,90,90                 | 0     |
| 57  | MG   | RA    | 3099 | 1/1   | 0.76 | 0.32 | 48,48,48,48                 | 0     |
| 57  | MG   | RA    | 3238 | 1/1   | 0.76 | 0.45 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3054 | 1/1   | 0.76 | 0.67 | 65,65,65,65                 | 0     |
| 57  | MG   | R5    | 101  | 1/1   | 0.76 | 1.48 | 291,291,291,291             | 0     |
| 57  | MG   | RA    | 3197 | 1/1   | 0.76 | 0.62 | 84,84,84,84                 | 0     |
| 57  | MG   | YA    | 3231 | 1/1   | 0.77 | 0.60 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3135 | 1/1   | 0.77 | 0.37 | 65,65,65,65                 | 0     |
| 57  | MG   | YA    | 3016 | 1/1   | 0.77 | 0.20 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3191 | 1/1   | 0.77 | 0.22 | 34,34,34,34                 | 0     |
| 57  | MG   | YA    | 3084 | 1/1   | 0.78 | 0.23 | 71,71,71,71                 | 0     |
| 57  | MG   | QA    | 1653 | 1/1   | 0.78 | 0.18 | 79,79,79,79                 | 0     |
| 57  | MG   | RA    | 3101 | 1/1   | 0.78 | 0.31 | 56,56,56,56                 | 0     |
| 57  | MG   | YA    | 3125 | 1/1   | 0.78 | 0.67 | 60,60,60,60                 | 0     |
| 57  | MG   | RA    | 3189 | 1/1   | 0.78 | 0.25 | 96,96,96,96                 | 0     |
| 57  | MG   | RA    | 3171 | 1/1   | 0.79 | 0.45 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3203 | 1/1   | 0.79 | 0.53 | 74,74,74,74                 | 0     |
| 57  | MG   | YA    | 3186 | 1/1   | 0.79 | 0.18 | 64,64,64,64                 | 0     |
| 57  | MG   | XA    | 1609 | 1/1   | 0.79 | 0.42 | 35,35,35,35                 | 0     |
| 57  | MG   | QA    | 1628 | 1/1   | 0.79 | 0.24 | 103,103,103,103             | 0     |
| 57  | MG   | RA    | 3158 | 1/1   | 0.79 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | QA    | 1660 | 1/1   | 0.79 | 0.32 | 193,193,193,193             | 0     |
| 57  | MG   | XB    | 301  | 1/1   | 0.79 | 0.59 | 87,87,87,87                 | 0     |
| 57  | MG   | YA    | 3167 | 1/1   | 0.79 | 0.31 | 69,69,69,69                 | 0     |
| 57  | MG   | YA    | 3190 | 1/1   | 0.79 | 0.57 | 51,51,51,51                 | 0     |
| 57  | MG   | XA    | 1648 | 1/1   | 0.79 | 0.21 | 75,75,75,75                 | 0     |
| 57  | MG   | YA    | 3150 | 1/1   | 0.80 | 0.36 | 114,114,114,114             | 0     |
| 57  | MG   | XA    | 1663 | 1/1   | 0.80 | 0.34 | 75,75,75,75                 | 0     |
| 57  | MG   | YA    | 3195 | 1/1   | 0.80 | 0.26 | 88,88,88,88                 | 0     |
| 57  | MG   | XA    | 1614 | 1/1   | 0.80 | 0.31 | 153,153,153,153             | 0     |
| 57  | MG   | YA    | 3237 | 1/1   | 0.80 | 0.54 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3214 | 1/1   | 0.80 | 0.44 | 244,244,244,244             | 0     |
| 57  | MG   | RA    | 3132 | 1/1   | 0.80 | 0.42 | 66,66,66,66                 | 0     |
| 57  | MG   | RA    | 3185 | 1/1   | 0.80 | 0.64 | 48,48,48,48                 | 0     |
| 57  | MG   | XM    | 201  | 1/1   | 0.80 | 0.45 | 173,173,173,173             | 0     |
| 57  | MG   | YA    | 3227 | 1/1   | 0.80 | 0.57 | 121,121,121,121             | 0     |
| 57  | MG   | YA    | 3256 | 1/1   | 0.80 | 0.31 | 128,128,128,128             | 0     |
| 57  | MG   | QA    | 1607 | 1/1   | 0.80 | 0.36 | 124,124,124,124             | 0     |
| 57  | MG   | YA    | 3071 | 1/1   | 0.80 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | XA    | 1659 | 1/1   | 0.80 | 0.50 | 102,102,102,102             | 0     |
| 57  | MG   | RA    | 3114 | 1/1   | 0.81 | 0.24 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3006 | 1/1   | 0.81 | 0.70 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3011 | 1/1   | 0.81 | 0.64 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3068 | 1/1   | 0.81 | 0.82 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3140 | 1/1   | 0.81 | 0.26 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3204 | 1/1   | 0.81 | 0.48 | 182,182,182,182             | 0     |
| 57  | MG   | QA    | 1640 | 1/1   | 0.82 | 0.36 | 78,78,78,78                 | 0     |
| 57  | MG   | RA    | 3025 | 1/1   | 0.82 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3190 | 1/1   | 0.82 | 0.37 | 107,107,107,107             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3123 | 1/1   | 0.82 | 0.28 | 55,55,55,55                 | 0     |
| 57  | MG   | RA    | 3245 | 1/1   | 0.82 | 0.83 | 128,128,128,128             | 0     |
| 57  | MG   | YA    | 3211 | 1/1   | 0.82 | 0.38 | 72,72,72,72                 | 0     |
| 57  | MG   | QA    | 1624 | 1/1   | 0.82 | 0.95 | 68,68,68,68                 | 0     |
| 57  | MG   | RA    | 3240 | 1/1   | 0.82 | 0.60 | 70,70,70,70                 | 0     |
| 57  | MG   | RA    | 3214 | 1/1   | 0.82 | 0.32 | 119,119,119,119             | 0     |
| 57  | MG   | YA    | 3177 | 1/1   | 0.82 | 0.60 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3246 | 1/1   | 0.83 | 0.28 | 198,198,198,198             | 0     |
| 57  | MG   | RA    | 3165 | 1/1   | 0.83 | 0.58 | 82,82,82,82                 | 0     |
| 57  | MG   | RA    | 3133 | 1/1   | 0.83 | 0.41 | 118,118,118,118             | 0     |
| 57  | MG   | QF    | 201  | 1/1   | 0.83 | 0.54 | 166,166,166,166             | 0     |
| 57  | MG   | QA    | 1618 | 1/1   | 0.83 | 0.52 | 47,47,47,47                 | 0     |
| 57  | MG   | XA    | 1638 | 1/1   | 0.83 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3144 | 1/1   | 0.83 | 0.26 | 62,62,62,62                 | 0     |
| 57  | MG   | YA    | 3273 | 1/1   | 0.83 | 0.86 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3263 | 1/1   | 0.83 | 0.58 | 60,60,60,60                 | 0     |
| 57  | MG   | YB    | 204  | 1/1   | 0.83 | 0.59 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3182 | 1/1   | 0.83 | 0.34 | 92,92,92,92                 | 0     |
| 57  | MG   | RA    | 3228 | 1/1   | 0.83 | 0.81 | 25,25,25,25                 | 0     |
| 57  | MG   | XA    | 1661 | 1/1   | 0.84 | 0.96 | 75,75,75,75                 | 0     |
| 57  | MG   | RA    | 3004 | 1/1   | 0.84 | 0.51 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3166 | 1/1   | 0.84 | 1.29 | 74,74,74,74                 | 0     |
| 57  | MG   | YA    | 3206 | 1/1   | 0.84 | 0.38 | 88,88,88,88                 | 0     |
| 57  | MG   | YA    | 3239 | 1/1   | 0.84 | 0.20 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3186 | 1/1   | 0.84 | 0.68 | 72,72,72,72                 | 0     |
| 57  | MG   | RA    | 3223 | 1/1   | 0.84 | 0.15 | 113,113,113,113             | 0     |
| 57  | MG   | RA    | 3130 | 1/1   | 0.84 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | RA    | 3001 | 1/1   | 0.84 | 0.82 | 44,44,44,44                 | 0     |
| 57  | MG   | QA    | 1615 | 1/1   | 0.84 | 0.54 | 88,88,88,88                 | 0     |
| 57  | MG   | RA    | 3177 | 1/1   | 0.84 | 0.81 | 72,72,72,72                 | 0     |
| 57  | MG   | XA    | 1629 | 1/1   | 0.85 | 0.42 | 104,104,104,104             | 0     |
| 57  | MG   | QA    | 1623 | 1/1   | 0.85 | 0.44 | 79,79,79,79                 | 0     |
| 57  | MG   | RA    | 3008 | 1/1   | 0.85 | 0.77 | 62,62,62,62                 | 0     |
| 57  | MG   | YA    | 3003 | 1/1   | 0.85 | 0.29 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3208 | 1/1   | 0.85 | 0.47 | 74,74,74,74                 | 0     |
| 57  | MG   | RA    | 3010 | 1/1   | 0.85 | 0.50 | 89,89,89,89                 | 0     |
| 57  | MG   | RA    | 3063 | 1/1   | 0.85 | 1.00 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3116 | 1/1   | 0.85 | 1.00 | 89,89,89,89                 | 0     |
| 57  | MG   | YA    | 3199 | 1/1   | 0.85 | 0.25 | 54,54,54,54                 | 0     |
| 57  | MG   | RA    | 3176 | 1/1   | 0.85 | 0.27 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3089 | 1/1   | 0.85 | 0.34 | 114,114,114,114             | 0     |
| 57  | MG   | RA    | 3188 | 1/1   | 0.85 | 0.42 | 103,103,103,103             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3230 | 1/1   | 0.85 | 0.82 | 92,92,92,92                 | 0     |
| 57  | MG   | XA    | 1631 | 1/1   | 0.85 | 0.23 | 68,68,68,68                 | 0     |
| 57  | MG   | YE    | 301  | 1/1   | 0.85 | 0.55 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3223 | 1/1   | 0.86 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3178 | 1/1   | 0.86 | 0.30 | 99,99,99,99                 | 0     |
| 57  | MG   | RA    | 3155 | 1/1   | 0.86 | 0.68 | 71,71,71,71                 | 0     |
| 57  | MG   | XA    | 1645 | 1/1   | 0.86 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3173 | 1/1   | 0.86 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1620 | 1/1   | 0.86 | 0.26 | 80,80,80,80                 | 0     |
| 57  | MG   | XA    | 1649 | 1/1   | 0.86 | 0.28 | 61,61,61,61                 | 0     |
| 57  | MG   | YA    | 3133 | 1/1   | 0.86 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3265 | 1/1   | 0.86 | 0.37 | 41,41,41,41                 | 0     |
| 57  | MG   | XA    | 1669 | 1/1   | 0.86 | 0.28 | 155,155,155,155             | 0     |
| 57  | MG   | YA    | 3219 | 1/1   | 0.86 | 0.50 | 105,105,105,105             | 0     |
| 57  | MG   | YA    | 3137 | 1/1   | 0.87 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3234 | 1/1   | 0.87 | 0.38 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3267 | 1/1   | 0.87 | 0.65 | 59,59,59,59                 | 0     |
| 57  | MG   | XA    | 1655 | 1/1   | 0.87 | 0.80 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3217 | 1/1   | 0.87 | 0.42 | 76,76,76,76                 | 0     |
| 57  | MG   | RA    | 3168 | 1/1   | 0.87 | 0.65 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3082 | 1/1   | 0.87 | 0.66 | 61,61,61,61                 | 0     |
| 57  | MG   | YB    | 202  | 1/1   | 0.87 | 0.80 | 70,70,70,70                 | 0     |
| 57  | MG   | RA    | 3233 | 1/1   | 0.87 | 0.23 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3244 | 1/1   | 0.87 | 0.28 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3140 | 1/1   | 0.87 | 0.27 | 74,74,74,74                 | 0     |
| 57  | MG   | YA    | 3275 | 1/1   | 0.87 | 0.79 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3249 | 1/1   | 0.87 | 0.28 | 27,27,27,27                 | 0     |
| 57  | MG   | XX    | 101  | 1/1   | 0.87 | 0.39 | 64,64,64,64                 | 0     |
| 57  | MG   | YA    | 3185 | 1/1   | 0.87 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | RA    | 3116 | 1/1   | 0.87 | 0.28 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3143 | 1/1   | 0.88 | 0.33 | 69,69,69,69                 | 0     |
| 57  | MG   | YA    | 3164 | 1/1   | 0.88 | 0.31 | 72,72,72,72                 | 0     |
| 57  | MG   | RA    | 3050 | 1/1   | 0.88 | 0.36 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3229 | 1/1   | 0.88 | 0.36 | 88,88,88,88                 | 0     |
| 57  | MG   | RA    | 3193 | 1/1   | 0.88 | 0.21 | 87,87,87,87                 | 0     |
| 57  | MG   | XA    | 1668 | 1/1   | 0.88 | 0.40 | 136,136,136,136             | 0     |
| 57  | MG   | RA    | 3243 | 1/1   | 0.88 | 0.64 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3082 | 1/1   | 0.88 | 0.23 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3067 | 1/1   | 0.88 | 0.31 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3147 | 1/1   | 0.88 | 0.28 | 120,120,120,120             | 0     |
| 57  | MG   | QA    | 1614 | 1/1   | 0.88 | 0.65 | 76,76,76,76                 | 0     |
| 57  | MG   | RA    | 3242 | 1/1   | 0.88 | 0.71 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3211 | 1/1   | 0.88 | 0.42 | 67,67,67,67                 | 0     |
| 57  | MG   | XA    | 1620 | 1/1   | 0.88 | 0.29 | 83,83,83,83                 | 0     |
| 57  | MG   | YA    | 3128 | 1/1   | 0.88 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3148 | 1/1   | 0.88 | 0.74 | 28,28,28,28                 | 0     |
| 57  | MG   | QA    | 1646 | 1/1   | 0.88 | 0.09 | 65,65,65,65                 | 0     |
| 57  | MG   | XA    | 1667 | 1/1   | 0.88 | 0.64 | 75,75,75,75                 | 0     |
| 57  | MG   | YA    | 3194 | 1/1   | 0.88 | 0.73 | 49,49,49,49                 | 0     |
| 57  | MG   | XA    | 1635 | 1/1   | 0.88 | 0.74 | 74,74,74,74                 | 0     |
| 57  | MG   | QA    | 1602 | 1/1   | 0.89 | 0.45 | 39,39,39,39                 | 0     |
| 57  | MG   | RA    | 3144 | 1/1   | 0.89 | 0.50 | 70,70,70,70                 | 0     |
| 57  | MG   | YA    | 3074 | 1/1   | 0.89 | 0.25 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3070 | 1/1   | 0.89 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3244 | 1/1   | 0.89 | 0.52 | 75,75,75,75                 | 0     |
| 57  | MG   | XA    | 1652 | 1/1   | 0.89 | 0.30 | 104,104,104,104             | 0     |
| 57  | MG   | RA    | 3181 | 1/1   | 0.89 | 0.21 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3200 | 1/1   | 0.89 | 0.44 | 58,58,58,58                 | 0     |
| 57  | MG   | XA    | 1656 | 1/1   | 0.89 | 0.60 | 89,89,89,89                 | 0     |
| 57  | MG   | YA    | 3094 | 1/1   | 0.89 | 0.60 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3266 | 1/1   | 0.89 | 0.54 | 64,64,64,64                 | 0     |
| 57  | MG   | RA    | 3148 | 1/1   | 0.89 | 0.33 | 90,90,90,90                 | 0     |
| 57  | MG   | YA    | 3191 | 1/1   | 0.89 | 0.20 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3041 | 1/1   | 0.89 | 0.39 | 35,35,35,35                 | 0     |
| 57  | MG   | QA    | 1647 | 1/1   | 0.89 | 0.29 | 67,67,67,67                 | 0     |
| 57  | MG   | YA    | 3174 | 1/1   | 0.89 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3044 | 1/1   | 0.89 | 0.74 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3075 | 1/1   | 0.89 | 0.74 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3195 | 1/1   | 0.89 | 0.23 | 102,102,102,102             | 0     |
| 57  | MG   | YA    | 3163 | 1/1   | 0.89 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | QA    | 1625 | 1/1   | 0.89 | 0.82 | 92,92,92,92                 | 0     |
| 57  | MG   | RA    | 3172 | 1/1   | 0.89 | 0.27 | 43,43,43,43                 | 0     |
| 57  | MG   | QA    | 1634 | 1/1   | 0.89 | 0.75 | 53,53,53,53                 | 0     |
| 57  | MG   | RA    | 3226 | 1/1   | 0.90 | 0.41 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3088 | 1/1   | 0.90 | 0.36 | 59,59,59,59                 | 0     |
| 57  | MG   | QA    | 1627 | 1/1   | 0.90 | 0.27 | 33,33,33,33                 | 0     |
| 57  | MG   | QA    | 1643 | 1/1   | 0.90 | 0.39 | 67,67,67,67                 | 0     |
| 57  | MG   | YA    | 3170 | 1/1   | 0.90 | 0.65 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3118 | 1/1   | 0.90 | 0.50 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3069 | 1/1   | 0.90 | 0.48 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3080 | 1/1   | 0.90 | 0.85 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3055 | 1/1   | 0.90 | 0.54 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3036 | 1/1   | 0.90 | 0.29 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3102 | 1/1   | 0.90 | 0.14 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3264 | 1/1   | 0.90 | 0.39 | 75,75,75,75                 | 0     |
| 57  | MG   | RA    | 3174 | 1/1   | 0.90 | 0.33 | 36,36,36,36                 | 0     |
| 57  | MG   | QA    | 1656 | 1/1   | 0.90 | 0.35 | 87,87,87,87                 | 0     |
| 57  | MG   | YA    | 3238 | 1/1   | 0.90 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3101 | 1/1   | 0.90 | 0.38 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3272 | 1/1   | 0.90 | 0.29 | 78,78,78,78                 | 0     |
| 57  | MG   | RA    | 3091 | 1/1   | 0.90 | 0.61 | 73,73,73,73                 | 0     |
| 57  | MG   | RA    | 3160 | 1/1   | 0.90 | 0.26 | 39,39,39,39                 | 0     |
| 57  | MG   | XA    | 1640 | 1/1   | 0.90 | 0.86 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3152 | 1/1   | 0.90 | 0.48 | 57,57,57,57                 | 0     |
| 57  | MG   | XA    | 1604 | 1/1   | 0.90 | 1.07 | 64,64,64,64                 | 0     |
| 57  | MG   | RA    | 3061 | 1/1   | 0.90 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | RA    | 3115 | 1/1   | 0.90 | 0.41 | 82,82,82,82                 | 0     |
| 57  | MG   | QA    | 1637 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | RA    | 3167 | 1/1   | 0.90 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | QA    | 1605 | 1/1   | 0.91 | 1.01 | 44,44,44,44                 | 0     |
| 57  | MG   | XA    | 1621 | 1/1   | 0.91 | 0.55 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3128 | 1/1   | 0.91 | 0.37 | 91,91,91,91                 | 0     |
| 57  | MG   | YA    | 3143 | 1/1   | 0.91 | 0.47 | 60,60,60,60                 | 0     |
| 57  | MG   | RA    | 3194 | 1/1   | 0.91 | 0.45 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3157 | 1/1   | 0.91 | 0.23 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3072 | 1/1   | 0.91 | 0.25 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3039 | 1/1   | 0.91 | 0.43 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3109 | 1/1   | 0.91 | 0.21 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3124 | 1/1   | 0.91 | 0.31 | 84,84,84,84                 | 0     |
| 57  | MG   | XA    | 1660 | 1/1   | 0.91 | 0.17 | 77,77,77,77                 | 0     |
| 57  | MG   | YA    | 3139 | 1/1   | 0.91 | 0.96 | 57,57,57,57                 | 0     |
| 57  | MG   | RA    | 3005 | 1/1   | 0.91 | 0.63 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3094 | 1/1   | 0.91 | 0.89 | 28,28,28,28                 | 0     |
| 57  | MG   | XV    | 102  | 1/1   | 0.91 | 0.30 | 61,61,61,61                 | 0     |
| 57  | MG   | QA    | 1613 | 1/1   | 0.91 | 0.64 | 57,57,57,57                 | 0     |
| 57  | MG   | YA    | 3105 | 1/1   | 0.91 | 0.32 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3111 | 1/1   | 0.91 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3196 | 1/1   | 0.91 | 0.27 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3073 | 1/1   | 0.91 | 0.32 | 70,70,70,70                 | 0     |
| 57  | MG   | YA    | 3151 | 1/1   | 0.91 | 0.26 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3041 | 1/1   | 0.91 | 0.34 | 32,32,32,32                 | 0     |
| 57  | MG   | RA    | 3200 | 1/1   | 0.91 | 0.31 | 76,76,76,76                 | 0     |
| 57  | MG   | YA    | 3024 | 1/1   | 0.91 | 0.47 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3232 | 1/1   | 0.91 | 0.33 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3047 | 1/1   | 0.91 | 0.59 | 26,26,26,26                 | 0     |
| 57  | MG   | QA    | 1658 | 1/1   | 0.91 | 0.34 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3270 | 1/1   | 0.91 | 0.83 | 57,57,57,57                 | 0     |
| 57  | MG   | XA    | 1671 | 1/1   | 0.91 | 0.28 | 76,76,76,76                 | 0     |
| 57  | MG   | YA    | 3037 | 1/1   | 0.91 | 0.37 | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1601 | 1/1   | 0.91 | 0.36 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3277 | 1/1   | 0.91 | 0.37 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3170 | 1/1   | 0.91 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | QY    | 101  | 1/1   | 0.91 | 0.18 | 83,83,83,83                 | 0     |
| 57  | MG   | YD    | 301  | 1/1   | 0.91 | 0.33 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3257 | 1/1   | 0.91 | 0.88 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3251 | 1/1   | 0.92 | 1.05 | 52,52,52,52                 | 0     |
| 57  | MG   | QA    | 1652 | 1/1   | 0.92 | 0.81 | 77,77,77,77                 | 0     |
| 57  | MG   | RA    | 3184 | 1/1   | 0.92 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | YE    | 302  | 1/1   | 0.92 | 0.35 | 31,31,31,31                 | 0     |
| 57  | MG   | QA    | 1654 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3162 | 1/1   | 0.92 | 0.14 | 72,72,72,72                 | 0     |
| 57  | MG   | YA    | 3019 | 1/1   | 0.92 | 0.46 | 25,25,25,25                 | 0     |
| 57  | MG   | QA    | 1641 | 1/1   | 0.92 | 0.20 | 76,76,76,76                 | 0     |
| 57  | MG   | XA    | 1647 | 1/1   | 0.92 | 0.42 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3173 | 1/1   | 0.92 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3134 | 1/1   | 0.92 | 0.29 | 39,39,39,39                 | 0     |
| 57  | MG   | RA    | 3026 | 1/1   | 0.92 | 0.78 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3115 | 1/1   | 0.92 | 0.31 | 64,64,64,64                 | 0     |
| 57  | MG   | YA    | 3242 | 1/1   | 0.92 | 0.87 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3166 | 1/1   | 0.92 | 0.84 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3175 | 1/1   | 0.92 | 0.53 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3278 | 1/1   | 0.92 | 0.26 | 85,85,85,85                 | 0     |
| 57  | MG   | YA    | 3065 | 1/1   | 0.92 | 0.27 | 53,53,53,53                 | 0     |
| 57  | MG   | XV    | 103  | 1/1   | 0.92 | 1.07 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3160 | 1/1   | 0.92 | 0.19 | 89,89,89,89                 | 0     |
| 57  | MG   | YA    | 3261 | 1/1   | 0.92 | 0.62 | 70,70,70,70                 | 0     |
| 57  | MG   | YA    | 3218 | 1/1   | 0.92 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | YA    | 3202 | 1/1   | 0.92 | 0.30 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3212 | 1/1   | 0.92 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1612 | 1/1   | 0.92 | 0.45 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3230 | 1/1   | 0.92 | 0.23 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3262 | 1/1   | 0.92 | 0.63 | 63,63,63,63                 | 0     |
| 57  | MG   | YA    | 3180 | 1/1   | 0.92 | 0.28 | 79,79,79,79                 | 0     |
| 57  | MG   | QA    | 1631 | 1/1   | 0.92 | 0.40 | 72,72,72,72                 | 0     |
| 58  | PAR  | QA    | 1667 | 42/42 | 0.92 | 0.20 | 72,72,72,72                 | 0     |
| 57  | MG   | RA    | 3097 | 1/1   | 0.92 | 0.52 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3150 | 1/1   | 0.92 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | XA    | 1619 | 1/1   | 0.92 | 0.37 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3039 | 1/1   | 0.92 | 0.29 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3006 | 1/1   | 0.92 | 0.48 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3184 | 1/1   | 0.92 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | XA    | 1630 | 1/1   | 0.92 | 0.53 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3047 | 1/1   | 0.92 | 0.46 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3235 | 1/1   | 0.92 | 0.35 | 63,63,63,63                 | 0     |
| 57  | MG   | QA    | 1662 | 1/1   | 0.92 | 0.19 | 100,100,100,100             | 0     |
| 57  | MG   | QA    | 1666 | 1/1   | 0.92 | 0.50 | 57,57,57,57                 | 0     |
| 57  | MG   | YA    | 3176 | 1/1   | 0.92 | 0.27 | 106,106,106,106             | 0     |
| 57  | MG   | RA    | 3112 | 1/1   | 0.92 | 0.33 | 78,78,78,78                 | 0     |
| 57  | MG   | YA    | 3246 | 1/1   | 0.92 | 0.52 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3088 | 1/1   | 0.92 | 0.35 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3240 | 1/1   | 0.92 | 0.86 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3203 | 1/1   | 0.93 | 0.24 | 139,139,139,139             | 0     |
| 57  | MG   | YA    | 3045 | 1/1   | 0.93 | 0.51 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3188 | 1/1   | 0.93 | 0.43 | 39,39,39,39                 | 0     |
| 57  | MG   | RA    | 3056 | 1/1   | 0.93 | 0.43 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3213 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3138 | 1/1   | 0.93 | 0.50 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3131 | 1/1   | 0.93 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | XA    | 1625 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | XA    | 1657 | 1/1   | 0.93 | 0.59 | 65,65,65,65                 | 0     |
| 57  | MG   | YA    | 3048 | 1/1   | 0.93 | 0.39 | 58,58,58,58                 | 0     |
| 57  | MG   | QA    | 1657 | 1/1   | 0.93 | 0.43 | 112,112,112,112             | 0     |
| 58  | PAR  | XA    | 1672 | 42/42 | 0.93 | 0.26 | 66,66,66,66                 | 0     |
| 57  | MG   | YA    | 3147 | 1/1   | 0.93 | 0.21 | 75,75,75,75                 | 0     |
| 57  | MG   | YA    | 3063 | 1/1   | 0.93 | 0.40 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3216 | 1/1   | 0.93 | 0.18 | 72,72,72,72                 | 0     |
| 57  | MG   | YA    | 3030 | 1/1   | 0.93 | 0.67 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3181 | 1/1   | 0.93 | 0.22 | 32,32,32,32                 | 0     |
| 57  | MG   | XA    | 1639 | 1/1   | 0.93 | 0.10 | 71,71,71,71                 | 0     |
| 57  | MG   | QA    | 1609 | 1/1   | 0.93 | 0.11 | 154,154,154,154             | 0     |
| 57  | MG   | YA    | 3183 | 1/1   | 0.93 | 0.63 | 67,67,67,67                 | 0     |
| 57  | MG   | RB    | 201  | 1/1   | 0.93 | 0.13 | 79,79,79,79                 | 0     |
| 57  | MG   | YA    | 3130 | 1/1   | 0.93 | 0.27 | 84,84,84,84                 | 0     |
| 57  | MG   | RA    | 3227 | 1/1   | 0.93 | 1.24 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3031 | 1/1   | 0.93 | 0.50 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3045 | 1/1   | 0.93 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3076 | 1/1   | 0.93 | 0.48 | 28,28,28,28                 | 0     |
| 59  | ZN   | R5    | 102  | 1/1   | 0.93 | 0.07 | 306,306,306,306             | 0     |
| 57  | MG   | YA    | 3131 | 1/1   | 0.93 | 0.69 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3076 | 1/1   | 0.93 | 0.69 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RP    | 202  | 1/1   | 0.93 | 0.46 | 64,64,64,64                 | 0     |
| 57  | MG   | YB    | 203  | 1/1   | 0.93 | 0.30 | 91,91,91,91                 | 0     |
| 57  | MG   | RA    | 3180 | 1/1   | 0.93 | 0.16 | 86,86,86,86                 | 0     |
| 57  | MG   | RA    | 3078 | 1/1   | 0.93 | 0.72 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3053 | 1/1   | 0.93 | 0.62 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3048 | 1/1   | 0.93 | 0.36 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3252 | 1/1   | 0.93 | 0.38 | 42,42,42,42                 | 0     |
| 57  | MG   | Y5    | 101  | 1/1   | 0.93 | 1.04 | 162,162,162,162             | 0     |
| 57  | MG   | XA    | 1658 | 1/1   | 0.93 | 0.53 | 101,101,101,101             | 0     |
| 57  | MG   | YA    | 3099 | 1/1   | 0.93 | 0.55 | 32,32,32,32                 | 0     |
| 57  | MG   | QV    | 102  | 1/1   | 0.93 | 0.24 | 69,69,69,69                 | 0     |
| 57  | MG   | QA    | 1616 | 1/1   | 0.93 | 0.20 | 81,81,81,81                 | 0     |
| 57  | MG   | YA    | 3145 | 1/1   | 0.93 | 0.20 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3113 | 1/1   | 0.94 | 0.32 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3104 | 1/1   | 0.94 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3056 | 1/1   | 0.94 | 0.24 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3231 | 1/1   | 0.94 | 0.63 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3009 | 1/1   | 0.94 | 0.36 | 68,68,68,68                 | 0     |
| 57  | MG   | YA    | 3002 | 1/1   | 0.94 | 0.47 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3075 | 1/1   | 0.94 | 0.25 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3271 | 1/1   | 0.94 | 1.04 | 84,84,84,84                 | 0     |
| 57  | MG   | RA    | 3028 | 1/1   | 0.94 | 0.41 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3077 | 1/1   | 0.94 | 0.32 | 32,32,32,32                 | 0     |
| 57  | MG   | QA    | 1665 | 1/1   | 0.94 | 0.47 | 82,82,82,82                 | 0     |
| 57  | MG   | QA    | 1635 | 1/1   | 0.94 | 0.28 | 58,58,58,58                 | 0     |
| 57  | MG   | YA    | 3110 | 1/1   | 0.94 | 0.28 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3046 | 1/1   | 0.94 | 0.63 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3066 | 1/1   | 0.94 | 0.27 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3221 | 1/1   | 0.94 | 0.39 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3084 | 1/1   | 0.94 | 0.35 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3205 | 1/1   | 0.94 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3276 | 1/1   | 0.94 | 0.40 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3142 | 1/1   | 0.94 | 0.72 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3241 | 1/1   | 0.94 | 0.35 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3149 | 1/1   | 0.94 | 0.26 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3269 | 1/1   | 0.94 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | RA    | 3046 | 1/1   | 0.94 | 0.73 | 35,35,35,35                 | 0     |
| 57  | MG   | XA    | 1641 | 1/1   | 0.94 | 0.38 | 74,74,74,74                 | 0     |
| 57  | MG   | YA    | 3015 | 1/1   | 0.94 | 0.59 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3064 | 1/1   | 0.94 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | XA    | 1633 | 1/1   | 0.94 | 0.31 | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3043 | 1/1   | 0.94 | 0.22 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | QA    | 1621 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3027 | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3142 | 1/1   | 0.94 | 0.30 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3260 | 1/1   | 0.94 | 0.54 | 67,67,67,67                 | 0     |
| 57  | MG   | RA    | 3019 | 1/1   | 0.94 | 0.34 | 61,61,61,61                 | 0     |
| 57  | MG   | RA    | 3053 | 1/1   | 0.94 | 0.46 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3168 | 1/1   | 0.94 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | YA    | 3172 | 1/1   | 0.94 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | RA    | 3055 | 1/1   | 0.94 | 0.77 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3129 | 1/1   | 0.94 | 0.64 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3043 | 1/1   | 0.94 | 0.82 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3096 | 1/1   | 0.94 | 0.76 | 53,53,53,53                 | 0     |
| 57  | MG   | RE    | 301  | 1/1   | 0.94 | 0.29 | 58,58,58,58                 | 0     |
| 57  | MG   | YA    | 3091 | 1/1   | 0.95 | 0.21 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3120 | 1/1   | 0.95 | 0.32 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3192 | 1/1   | 0.95 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | YA    | 3232 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3105 | 1/1   | 0.95 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3004 | 1/1   | 0.95 | 0.41 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3015 | 1/1   | 0.95 | 0.50 | 26,26,26,26                 | 0     |
| 57  | MG   | QA    | 1619 | 1/1   | 0.95 | 0.26 | 68,68,68,68                 | 0     |
| 57  | MG   | YA    | 3122 | 1/1   | 0.95 | 0.70 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3192 | 1/1   | 0.95 | 0.29 | 250,250,250,250             | 0     |
| 57  | MG   | QA    | 1661 | 1/1   | 0.95 | 0.09 | 126,126,126,126             | 0     |
| 57  | MG   | QA    | 1650 | 1/1   | 0.95 | 0.46 | 91,91,91,91                 | 0     |
| 57  | MG   | RA    | 3122 | 1/1   | 0.95 | 0.89 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3241 | 1/1   | 0.95 | 0.25 | 54,54,54,54                 | 0     |
| 57  | MG   | RA    | 3135 | 1/1   | 0.95 | 0.55 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3093 | 1/1   | 0.95 | 0.49 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3013 | 1/1   | 0.95 | 0.87 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3207 | 1/1   | 0.95 | 0.24 | 116,116,116,116             | 0     |
| 57  | MG   | RA    | 3124 | 1/1   | 0.95 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | YA    | 3208 | 1/1   | 0.95 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | XA    | 1603 | 1/1   | 0.95 | 0.42 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3210 | 1/1   | 0.95 | 0.41 | 74,74,74,74                 | 0     |
| 57  | MG   | RA    | 3051 | 1/1   | 0.95 | 0.38 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3085 | 1/1   | 0.95 | 0.44 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3081 | 1/1   | 0.95 | 0.35 | 28,28,28,28                 | 0     |
| 57  | MG   | QA    | 1668 | 1/1   | 0.95 | 0.09 | 101,101,101,101             | 0     |
| 57  | MG   | XA    | 1605 | 1/1   | 0.95 | 0.65 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3054 | 1/1   | 0.95 | 0.22 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3154 | 1/1   | 0.95 | 0.43 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3126 | 1/1   | 0.95 | 0.22 | 58,58,58,58                 | 0     |
| 57  | MG   | XY    | 101  | 1/1   | 0.95 | 0.17 | 74,74,74,74                 | 0     |
| 57  | MG   | XA    | 1643 | 1/1   | 0.95 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | QA    | 1645 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3087 | 1/1   | 0.95 | 0.44 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3114 | 1/1   | 0.95 | 0.26 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3033 | 1/1   | 0.95 | 0.47 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3003 | 1/1   | 0.95 | 0.47 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3071 | 1/1   | 0.95 | 0.22 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3237 | 1/1   | 0.95 | 0.42 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3222 | 1/1   | 0.95 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | XA    | 1665 | 1/1   | 0.95 | 0.52 | 74,74,74,74                 | 0     |
| 59  | ZN   | QN    | 101  | 1/1   | 0.95 | 0.12 | 127,127,127,127             | 0     |
| 57  | MG   | YA    | 3060 | 1/1   | 0.95 | 0.42 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3141 | 1/1   | 0.95 | 0.37 | 45,45,45,45                 | 0     |
| 59  | ZN   | QD    | 301  | 1/1   | 0.95 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3100 | 1/1   | 0.95 | 0.48 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3086 | 1/1   | 0.95 | 0.77 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3040 | 1/1   | 0.95 | 0.54 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3205 | 1/1   | 0.95 | 0.30 | 78,78,78,78                 | 0     |
| 57  | MG   | XA    | 1654 | 1/1   | 0.95 | 0.45 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3123 | 1/1   | 0.95 | 0.29 | 51,51,51,51                 | 0     |
| 57  | MG   | Y7    | 101  | 1/1   | 0.95 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | XA    | 1606 | 1/1   | 0.95 | 0.54 | 76,76,76,76                 | 0     |
| 57  | MG   | RA    | 3134 | 1/1   | 0.95 | 0.33 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3121 | 1/1   | 0.95 | 0.23 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3136 | 1/1   | 0.95 | 0.24 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3020 | 1/1   | 0.95 | 0.82 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3117 | 1/1   | 0.95 | 0.29 | 84,84,84,84                 | 0     |
| 57  | MG   | RA    | 3057 | 1/1   | 0.95 | 0.46 | 133,133,133,133             | 0     |
| 57  | MG   | RA    | 3169 | 1/1   | 0.95 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3145 | 1/1   | 0.95 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3021 | 1/1   | 0.95 | 0.29 | 29,29,29,29                 | 0     |
| 57  | MG   | XA    | 1642 | 1/1   | 0.95 | 0.54 | 41,41,41,41                 | 0     |
| 57  | MG   | QA    | 1663 | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3187 | 1/1   | 0.96 | 0.33 | 49,49,49,49                 | 0     |
| 57  | MG   | XA    | 1616 | 1/1   | 0.96 | 0.27 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3198 | 1/1   | 0.96 | 0.15 | 86,86,86,86                 | 0     |
| 57  | MG   | RA    | 3102 | 1/1   | 0.96 | 0.48 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3222 | 1/1   | 0.96 | 0.38 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3209 | 1/1   | 0.96 | 0.38 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3202 | 1/1   | 0.96 | 0.67 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3070 | 1/1   | 0.96 | 0.34 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3062 | 1/1   | 0.96 | 0.81 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3087 | 1/1   | 0.96 | 0.49 | 54,54,54,54                 | 0     |
| 57  | MG   | QA    | 1611 | 1/1   | 0.96 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3029 | 1/1   | 0.96 | 0.27 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3052 | 1/1   | 0.96 | 0.56 | 41,41,41,41                 | 0     |
| 57  | MG   | YA    | 3059 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3089 | 1/1   | 0.96 | 0.48 | 53,53,53,53                 | 0     |
| 57  | MG   | RA    | 3049 | 1/1   | 0.96 | 0.43 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3083 | 1/1   | 0.96 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3199 | 1/1   | 0.96 | 0.68 | 56,56,56,56                 | 0     |
| 57  | MG   | YA    | 3032 | 1/1   | 0.96 | 0.29 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3027 | 1/1   | 0.96 | 0.20 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3108 | 1/1   | 0.96 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3018 | 1/1   | 0.96 | 0.53 | 48,48,48,48                 | 0     |
| 57  | MG   | XA    | 1627 | 1/1   | 0.96 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3198 | 1/1   | 0.96 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3100 | 1/1   | 0.96 | 0.28 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3058 | 1/1   | 0.96 | 0.42 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3095 | 1/1   | 0.96 | 0.43 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3016 | 1/1   | 0.96 | 0.47 | 39,39,39,39                 | 0     |
| 57  | MG   | XA    | 1636 | 1/1   | 0.96 | 0.28 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3096 | 1/1   | 0.96 | 0.27 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3031 | 1/1   | 0.96 | 0.73 | 37,37,37,37                 | 0     |
| 57  | MG   | QA    | 1659 | 1/1   | 0.96 | 0.40 | 70,70,70,70                 | 0     |
| 57  | MG   | YA    | 3255 | 1/1   | 0.96 | 0.64 | 34,34,34,34                 | 0     |
| 57  | MG   | YA    | 3107 | 1/1   | 0.96 | 0.49 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3042 | 1/1   | 0.96 | 0.42 | 45,45,45,45                 | 0     |
| 57  | MG   | XA    | 1637 | 1/1   | 0.96 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3182 | 1/1   | 0.96 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3009 | 1/1   | 0.96 | 0.62 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3022 | 1/1   | 0.96 | 0.38 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3163 | 1/1   | 0.96 | 0.28 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3040 | 1/1   | 0.96 | 0.26 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3093 | 1/1   | 0.96 | 0.53 | 34,34,34,34                 | 0     |
| 57  | MG   | RB    | 202  | 1/1   | 0.96 | 0.08 | 100,100,100,100             | 0     |
| 57  | MG   | RA    | 3137 | 1/1   | 0.96 | 0.33 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3146 | 1/1   | 0.96 | 0.17 | 137,137,137,137             | 0     |
| 57  | MG   | QA    | 1617 | 1/1   | 0.96 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3086 | 1/1   | 0.96 | 0.52 | 28,28,28,28                 | 0     |
| 57  | MG   | XA    | 1624 | 1/1   | 0.96 | 0.58 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3085 | 1/1   | 0.96 | 0.32 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3193 | 1/1   | 0.97 | 0.42 | 230,230,230,230             | 0     |
| 57  | MG   | YA    | 3023 | 1/1   | 0.97 | 0.31 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3250 | 1/1   | 0.97 | 0.62 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3028 | 1/1   | 0.97 | 0.32 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3001 | 1/1   | 0.97 | 0.75 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3103 | 1/1   | 0.97 | 0.41 | 41,41,41,41                 | 0     |
| 57  | MG   | YA    | 3189 | 1/1   | 0.97 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3098 | 1/1   | 0.97 | 0.21 | 65,65,65,65                 | 0     |
| 57  | MG   | RA    | 3037 | 1/1   | 0.97 | 0.41 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3108 | 1/1   | 0.97 | 0.37 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3073 | 1/1   | 0.97 | 0.36 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3069 | 1/1   | 0.97 | 0.43 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3034 | 1/1   | 0.97 | 0.85 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3236 | 1/1   | 0.97 | 0.33 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3171 | 1/1   | 0.97 | 0.62 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3179 | 1/1   | 0.97 | 0.14 | 113,113,113,113             | 0     |
| 57  | MG   | QA    | 1622 | 1/1   | 0.97 | 0.20 | 103,103,103,103             | 0     |
| 57  | MG   | RP    | 201  | 1/1   | 0.97 | 0.19 | 166,166,166,166             | 0     |
| 59  | ZN   | Y9    | 300  | 1/1   | 0.97 | 0.08 | 101,101,101,101             | 0     |
| 57  | MG   | XA    | 1632 | 1/1   | 0.97 | 0.45 | 41,41,41,41                 | 0     |
| 57  | MG   | YA    | 3117 | 1/1   | 0.97 | 0.20 | 39,39,39,39                 | 0     |
| 57  | MG   | RA    | 3209 | 1/1   | 0.97 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | YA    | 3146 | 1/1   | 0.97 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | RA    | 3236 | 1/1   | 0.97 | 0.85 | 46,46,46,46                 | 0     |
| 57  | MG   | YA    | 3067 | 1/1   | 0.97 | 0.29 | 37,37,37,37                 | 0     |
| 57  | MG   | XA    | 1613 | 1/1   | 0.97 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | YB    | 205  | 1/1   | 0.97 | 0.19 | 231,231,231,231             | 0     |
| 57  | MG   | RA    | 3235 | 1/1   | 0.97 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3062 | 1/1   | 0.97 | 0.42 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3092 | 1/1   | 0.97 | 0.30 | 25,25,25,25                 | 0     |
| 57  | MG   | XA    | 1617 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3127 | 1/1   | 0.97 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | XA    | 1623 | 1/1   | 0.97 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3007 | 1/1   | 0.97 | 0.23 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3014 | 1/1   | 0.97 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | RA    | 3125 | 1/1   | 0.97 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | RA    | 3113 | 1/1   | 0.97 | 0.69 | 34,34,34,34                 | 0     |
| 57  | MG   | XA    | 1626 | 1/1   | 0.97 | 0.43 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3111 | 1/1   | 0.97 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3036 | 1/1   | 0.97 | 0.43 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3038 | 1/1   | 0.97 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3017 | 1/1   | 0.97 | 0.30 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3129 | 1/1   | 0.97 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | XA    | 1611 | 1/1   | 0.97 | 0.28 | 28,28,28,28                 | 0     |
| 57  | MG   | XA    | 1615 | 1/1   | 0.97 | 0.42 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3017 | 1/1   | 0.97 | 0.32 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3020 | 1/1   | 0.97 | 0.75 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3013 | 1/1   | 0.97 | 0.43 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3022 | 1/1   | 0.97 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | QA    | 1604 | 1/1   | 0.97 | 0.30 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3225 | 1/1   | 0.97 | 0.39 | 67,67,67,67                 | 0     |
| 57  | MG   | YA    | 3049 | 1/1   | 0.97 | 0.41 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3012 | 1/1   | 0.97 | 0.33 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3079 | 1/1   | 0.97 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3159 | 1/1   | 0.97 | 0.39 | 34,34,34,34                 | 0     |
| 57  | MG   | YA    | 3034 | 1/1   | 0.97 | 0.39 | 27,27,27,27                 | 0     |
| 57  | MG   | QV    | 101  | 1/1   | 0.97 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3078 | 1/1   | 0.97 | 0.47 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3011 | 1/1   | 0.97 | 0.42 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3247 | 1/1   | 0.97 | 1.06 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3038 | 1/1   | 0.97 | 0.29 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3098 | 1/1   | 0.97 | 0.57 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3220 | 1/1   | 0.97 | 0.55 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3051 | 1/1   | 0.97 | 0.46 | 26,26,26,26                 | 0     |
| 57  | MG   | RA    | 3110 | 1/1   | 0.97 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3120 | 1/1   | 0.97 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3018 | 1/1   | 0.97 | 0.55 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3021 | 1/1   | 0.97 | 0.38 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3245 | 1/1   | 0.97 | 0.53 | 25,25,25,25                 | 0     |
| 57  | MG   | YX    | 101  | 1/1   | 0.97 | 0.21 | 196,196,196,196             | 0     |
| 57  | MG   | YA    | 3033 | 1/1   | 0.97 | 0.54 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3095 | 1/1   | 0.97 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3109 | 1/1   | 0.97 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3081 | 1/1   | 0.97 | 1.05 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3106 | 1/1   | 0.97 | 0.52 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3226 | 1/1   | 0.97 | 0.16 | 74,74,74,74                 | 0     |
| 57  | MG   | QA    | 1642 | 1/1   | 0.97 | 0.36 | 56,56,56,56                 | 0     |
| 57  | MG   | RA    | 3074 | 1/1   | 0.98 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3059 | 1/1   | 0.98 | 0.34 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3090 | 1/1   | 0.98 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3187 | 1/1   | 0.98 | 0.41 | 73,73,73,73                 | 0     |
| 57  | MG   | XA    | 1610 | 1/1   | 0.98 | 0.29 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3010 | 1/1   | 0.98 | 0.48 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3060 | 1/1   | 0.98 | 0.26 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3183 | 1/1   | 0.98 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | YA    | 3066 | 1/1   | 0.98 | 0.73 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3119 | 1/1   | 0.98 | 0.43 | 76,76,76,76                 | 0     |
| 57  | MG   | YA    | 3162 | 1/1   | 0.98 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3077 | 1/1   | 0.98 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3104 | 1/1   | 0.98 | 0.44 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3112 | 1/1   | 0.98 | 0.27 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3119 | 1/1   | 0.98 | 0.32 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3029 | 1/1   | 0.98 | 0.76 | 39,39,39,39                 | 0     |
| 57  | MG   | QA    | 1606 | 1/1   | 0.98 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | YP    | 201  | 1/1   | 0.98 | 0.49 | 380,380,380,380             | 0     |
| 57  | MG   | XA    | 1618 | 1/1   | 0.98 | 0.32 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3080 | 1/1   | 0.98 | 0.81 | 75,75,75,75                 | 0     |
| 57  | MG   | RA    | 3207 | 1/1   | 0.98 | 0.28 | 156,156,156,156             | 0     |
| 57  | MG   | RA    | 3090 | 1/1   | 0.98 | 0.46 | 40,40,40,40                 | 0     |
| 57  | MG   | XV    | 101  | 1/1   | 0.98 | 0.28 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3014 | 1/1   | 0.98 | 0.39 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3050 | 1/1   | 0.98 | 0.35 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3024 | 1/1   | 0.98 | 0.31 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3097 | 1/1   | 0.98 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3052 | 1/1   | 0.98 | 0.27 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3035 | 1/1   | 0.98 | 0.53 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3106 | 1/1   | 0.98 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3154 | 1/1   | 0.98 | 0.20 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3248 | 1/1   | 0.98 | 0.32 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3107 | 1/1   | 0.98 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3253 | 1/1   | 0.98 | 0.90 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3026 | 1/1   | 0.98 | 0.98 | 30,30,30,30                 | 0     |
| 57  | MG   | QA    | 1610 | 1/1   | 0.98 | 0.25 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3030 | 1/1   | 0.98 | 0.27 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3079 | 1/1   | 0.98 | 0.26 | 26,26,26,26                 | 0     |
| 57  | MG   | XA    | 1602 | 1/1   | 0.98 | 0.27 | 36,36,36,36                 | 0     |
| 57  | MG   | QA    | 1636 | 1/1   | 0.98 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | QA    | 1608 | 1/1   | 0.98 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3058 | 1/1   | 0.98 | 0.29 | 49,49,49,49                 | 0     |
| 57  | MG   | XA    | 1644 | 1/1   | 0.98 | 0.32 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3215 | 1/1   | 0.98 | 0.37 | 61,61,61,61                 | 0     |
| 59  | ZN   | XN    | 101  | 1/1   | 0.98 | 0.16 | 76,76,76,76                 | 0     |
| 57  | MG   | YA    | 3057 | 1/1   | 0.98 | 0.79 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3035 | 1/1   | 0.98 | 0.51 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3042 | 1/1   | 0.98 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | QA    | 1630 | 1/1   | 0.98 | 0.14 | 101,101,101,101             | 0     |

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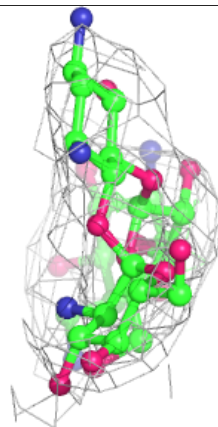
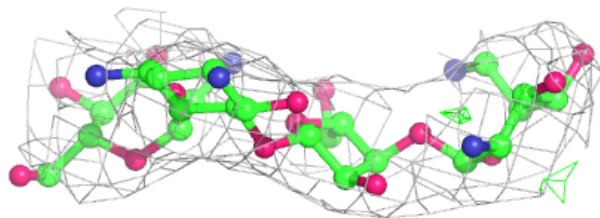
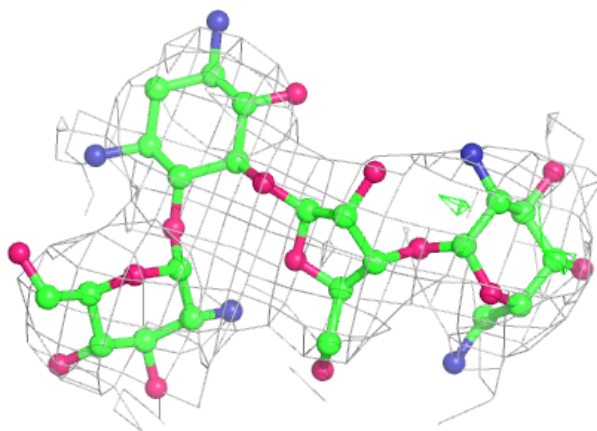
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | XA    | 1622 | 1/1   | 0.98 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3005 | 1/1   | 0.98 | 0.22 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3068 | 1/1   | 0.98 | 0.46 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3121 | 1/1   | 0.98 | 0.27 | 69,69,69,69                 | 0     |
| 57  | MG   | RP    | 203  | 1/1   | 0.98 | 0.18 | 381,381,381,381             | 0     |
| 57  | MG   | RA    | 3092 | 1/1   | 0.98 | 0.46 | 71,71,71,71                 | 0     |
| 57  | MG   | YA    | 3197 | 1/1   | 0.98 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3061 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3103 | 1/1   | 0.98 | 0.59 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3221 | 1/1   | 0.98 | 0.37 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3025 | 1/1   | 0.99 | 0.42 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3126 | 1/1   | 0.99 | 0.40 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3032 | 1/1   | 0.99 | 0.49 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3008 | 1/1   | 0.99 | 0.33 | 48,48,48,48                 | 0     |
| 57  | MG   | XA    | 1612 | 1/1   | 0.99 | 0.18 | 37,37,37,37                 | 0     |
| 59  | ZN   | XD    | 301  | 1/1   | 0.99 | 0.31 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3023 | 1/1   | 0.99 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | XA    | 1646 | 1/1   | 0.99 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3234 | 1/1   | 0.99 | 0.10 | 147,147,147,147             | 0     |
| 57  | MG   | QA    | 1648 | 1/1   | 0.99 | 0.07 | 93,93,93,93                 | 0     |
| 57  | MG   | RA    | 3065 | 1/1   | 0.99 | 0.41 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3083 | 1/1   | 0.99 | 0.54 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3064 | 1/1   | 0.99 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3268 | 1/1   | 0.99 | 0.29 | 66,66,66,66                 | 0     |
| 57  | MG   | RA    | 3204 | 1/1   | 0.99 | 0.20 | 167,167,167,167             | 0     |
| 57  | MG   | RA    | 3072 | 1/1   | 0.99 | 0.26 | 54,54,54,54                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

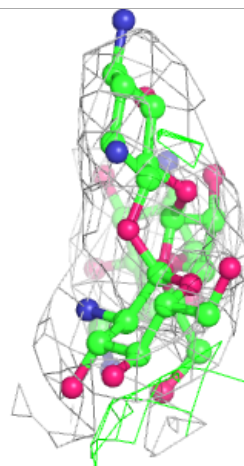
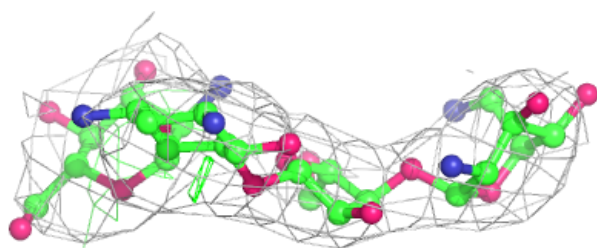
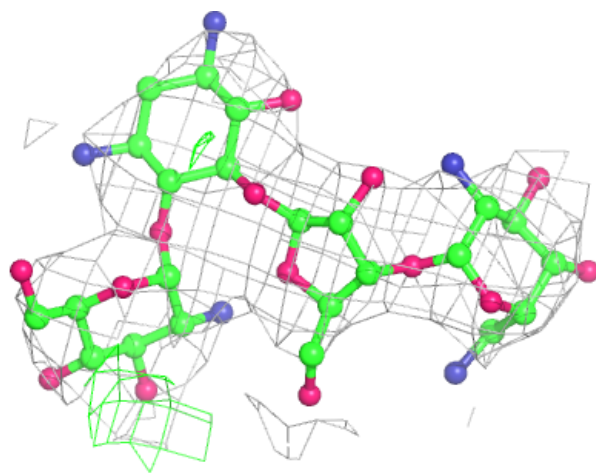
**Electron density around PAR QA 1667:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR XA 1672:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.