



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 PM UTC

PDB ID : 4LSK / pdb\_00004lsk  
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCG-G on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-07-22  
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

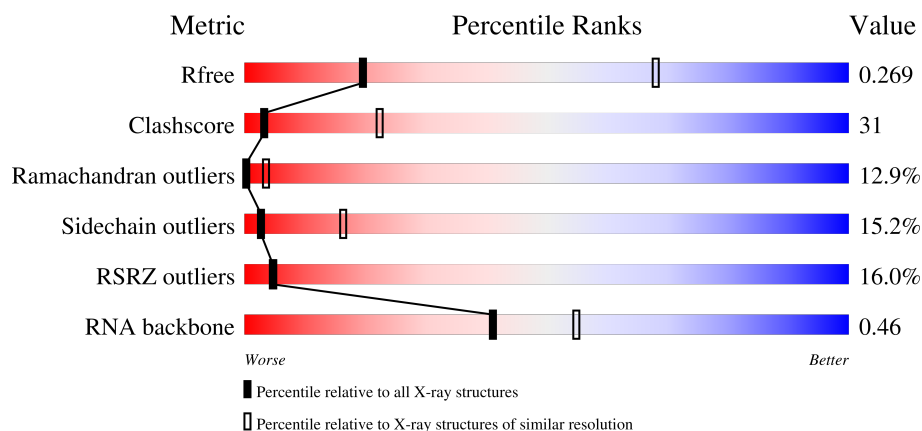
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1083 (3.52-3.44)                                      |
| Clashscore            | 190562                      | 1139 (3.52-3.44)                                      |
| Ramachandran outliers | 187476                      | 1111 (3.52-3.44)                                      |
| Sidechain outliers    | 187428                      | 1112 (3.52-3.44)                                      |
| RSRZ outliers         | 180081                      | 1082 (3.52-3.44)                                      |
| RNA backbone          | 3983                        | 1001 (3.94-3.02)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | QA    | 1522   |                  |
| 1   | XA    | 1522   |                  |
| 2   | QB    | 256    |                  |
| 2   | XB    | 256    |                  |

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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  | QY    | 17     |                  |
| 23  | XY    | 17     |                  |
| 24  | QX    | 25     |                  |
| 24  | XX    | 25     |                  |
| 25  | RA    | 2916   |                  |
| 25  | YA    | 2916   |                  |
| 26  | RB    | 122    |                  |
| 26  | YB    | 122    |                  |
| 27  | RD    | 276    |                  |
| 27  | YD    | 276    |                  |

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

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | R7    | 49     |                  |
| 53  | Y7    | 49     |                  |
| 54  | R8    | 65     |                  |
| 54  | Y8    | 65     |                  |
| 55  | R9    | 37     |                  |
| 55  | Y9    | 37     |                  |
| 56  | Z6    | 3      |                  |
| 56  | Z8    | 3      |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | RA    | 3120 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3082 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3085 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3122 | -         | -        | -       | X                |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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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.

| 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 S21.

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 23  | QY    | 15       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 323   | 144 | 58 | 106 | 15 |         |         |       |
| 23  | XY    | 15       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 323   | 144 | 58 | 106 | 15 |         |         |       |

- Molecule 24 is a RNA chain called A-site ASL SufA6.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 24  | QX    | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 173   | 77 | 33 | 55 | 8 |         |         |       |
| 24  | XX    | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 173   | 77 | 33 | 55 | 8 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 56  | Z6    | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 74    | 40 | 13 | 19 | 2 |         |         |       |
| 56  | Z8    | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 74    | 40 | 13 | 19 | 2 |         |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

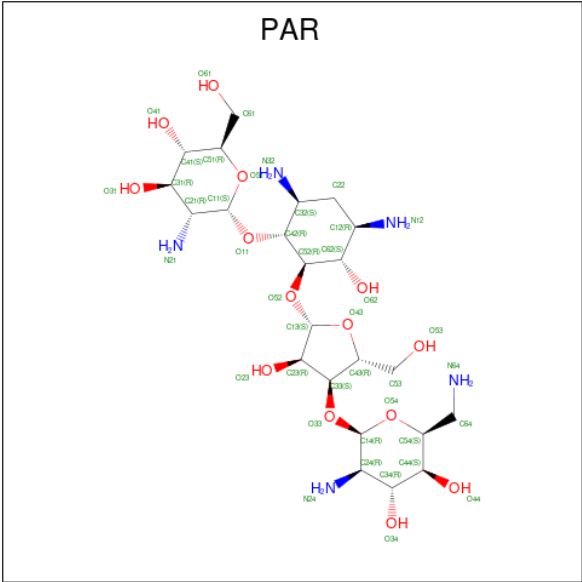
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | QA    | 65       | Total | Mg | 0       | 0       |
|     |       |          | 65    | 65 |         |         |
| 57  | QF    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | QH    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | QM    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | QV    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | QX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RA    | 241      | Total<br>241 | Mg<br>241 | 0       | 0       |
| 57  | RB    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | RD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | RF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | R0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | R5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XA    | 74       | Total<br>74  | Mg<br>74  | 0       | 0       |
| 57  | YA    | 268      | Total<br>268 | Mg<br>268 | 0       | 0       |
| 57  | YB    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | YE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | YP    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | Y0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | Y5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 58 is PAROMOMYCIN (CCD ID: 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 |         |         |

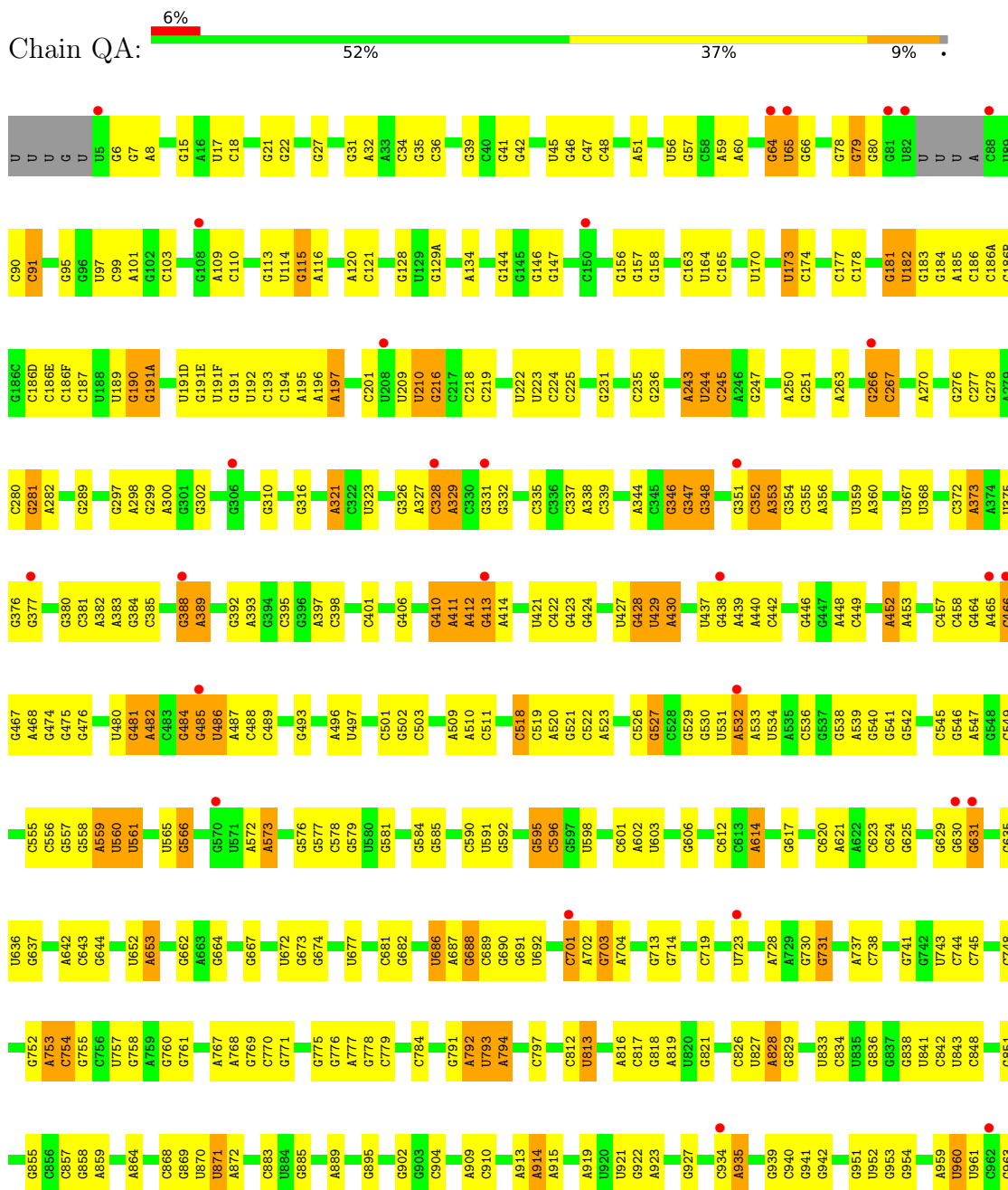
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

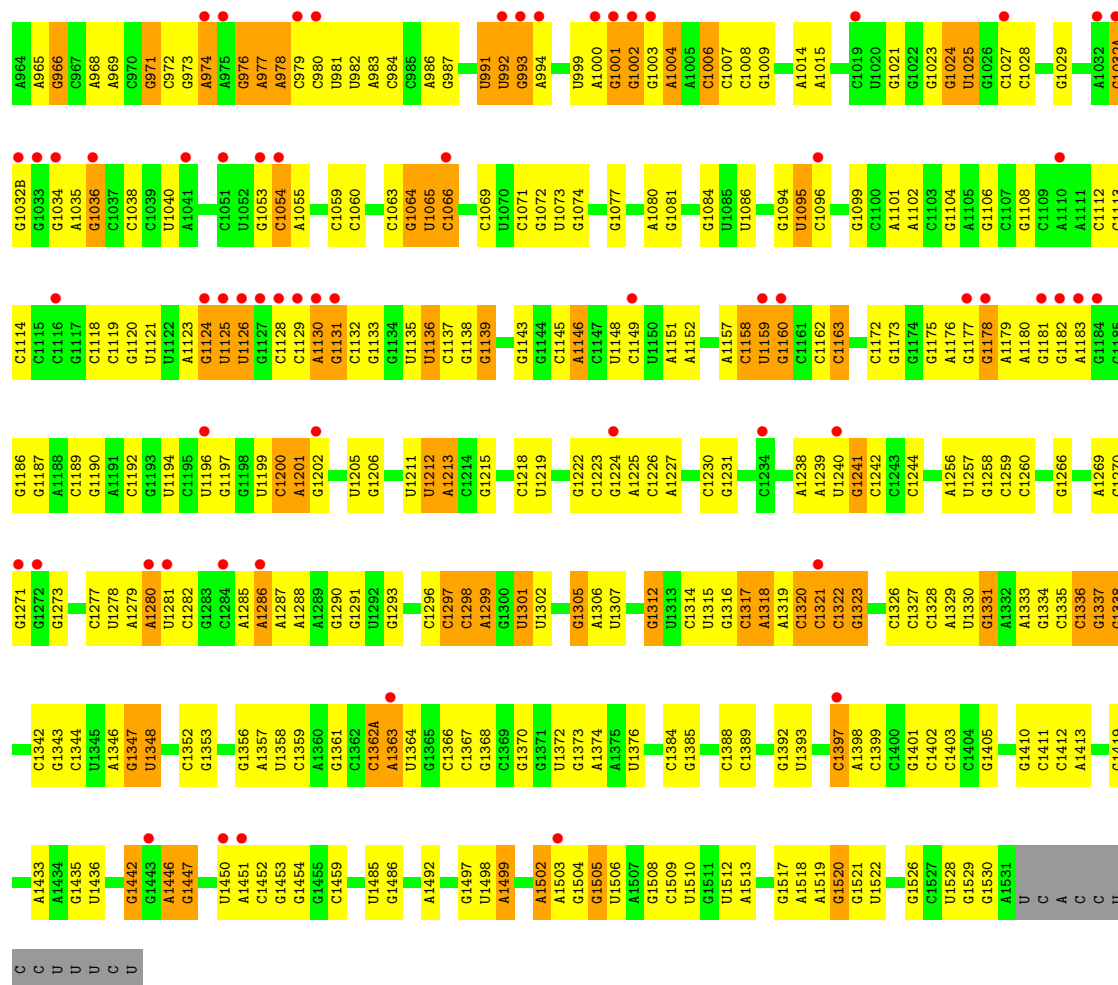
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | QD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | QN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | R9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | Y9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

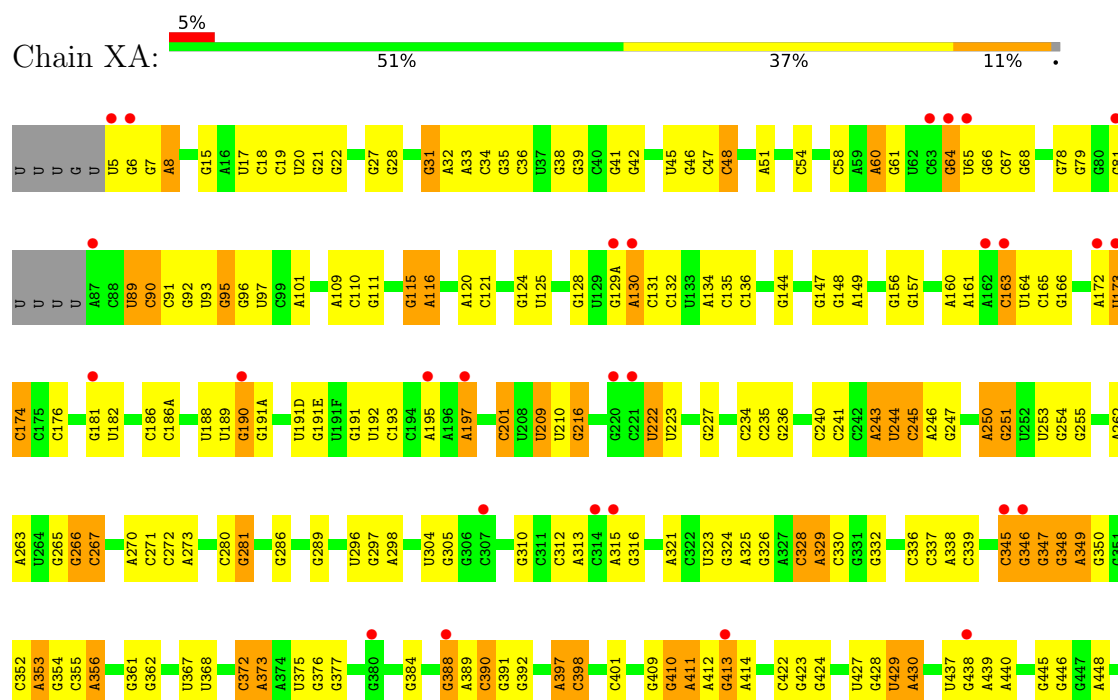
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

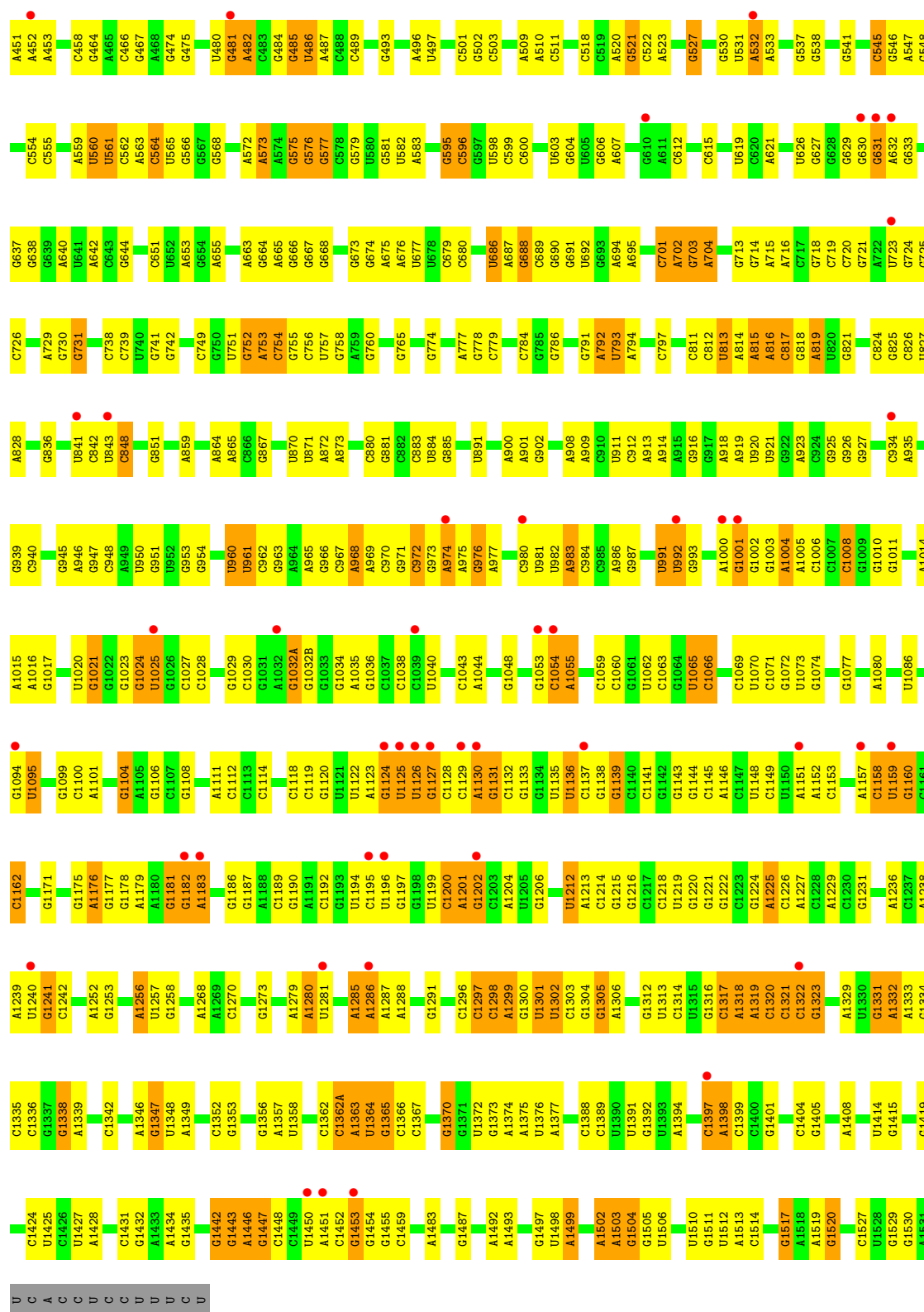
- Molecule 1: 16S rRNA



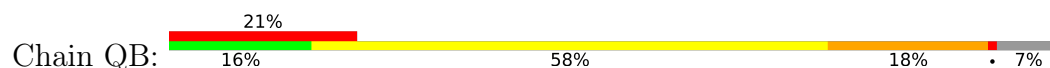


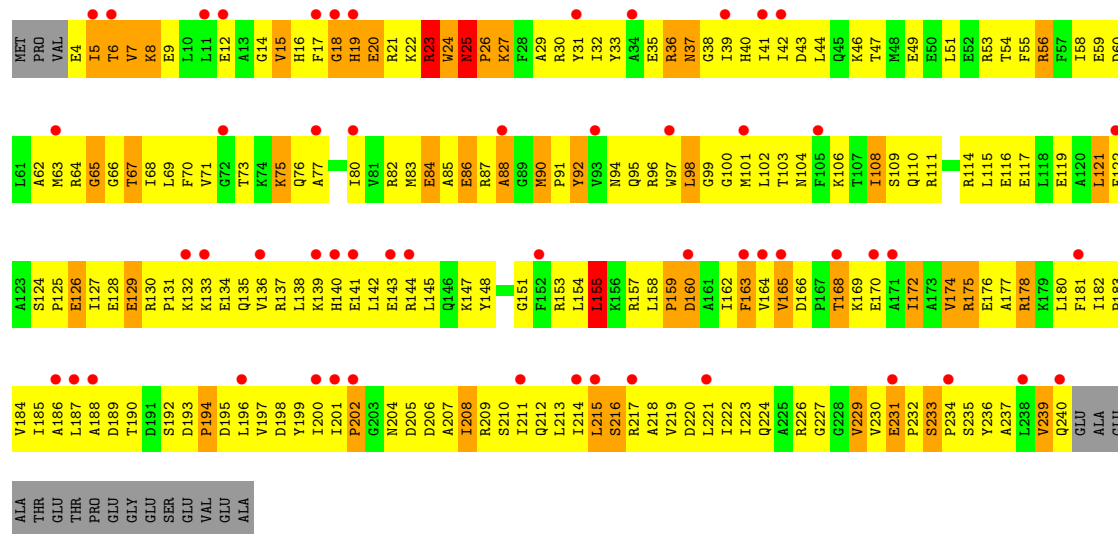
- Molecule 1: 16S rRNA



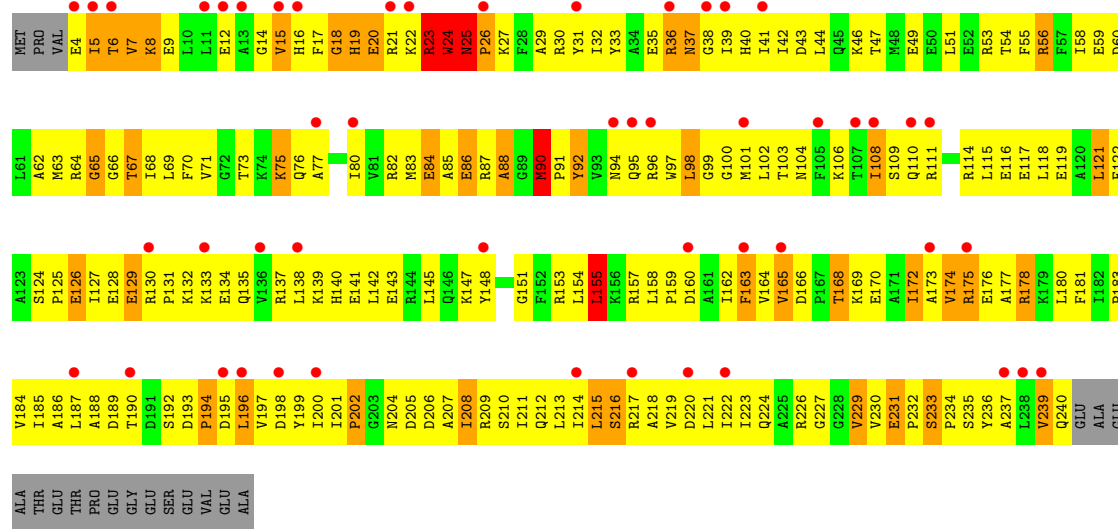
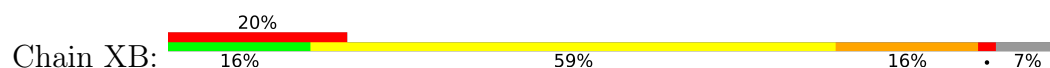


- Molecule 2: 30S ribosomal protein S2

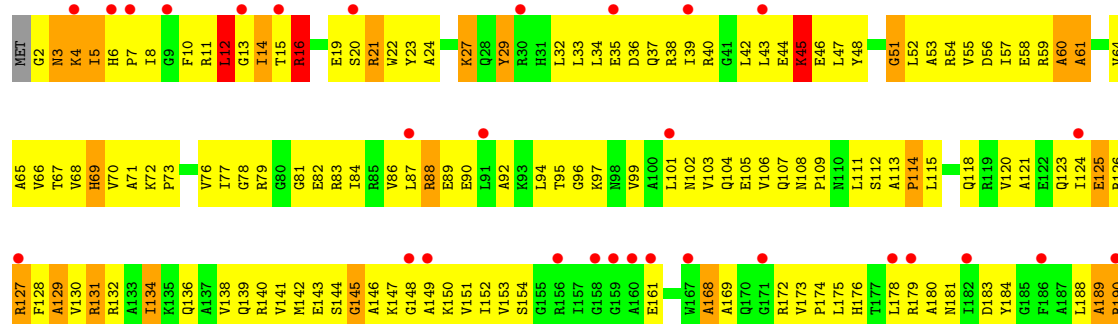




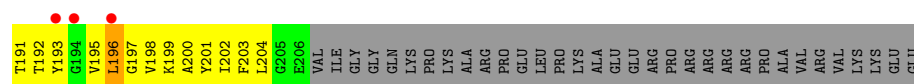
• Molecule 2: 30S ribosomal protein S2



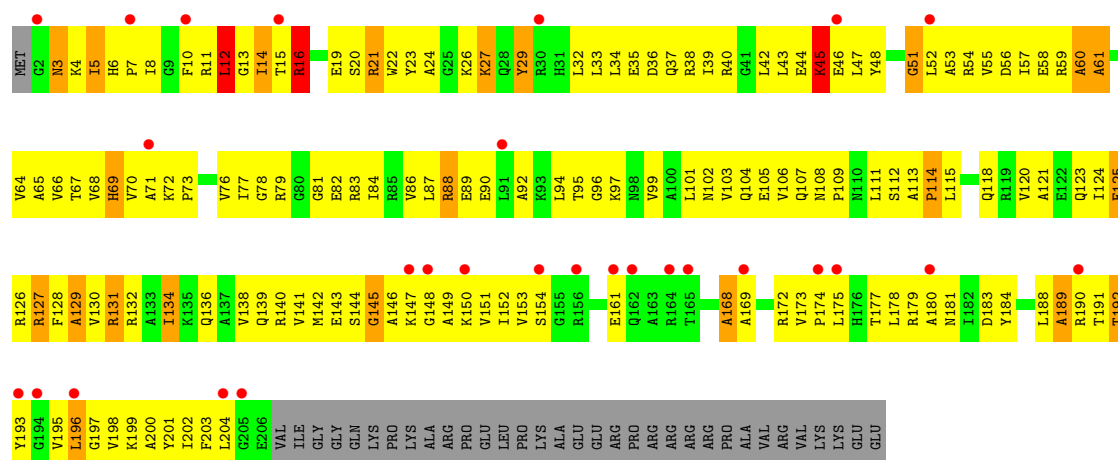
• Molecule 3: 30S ribosomal protein S3



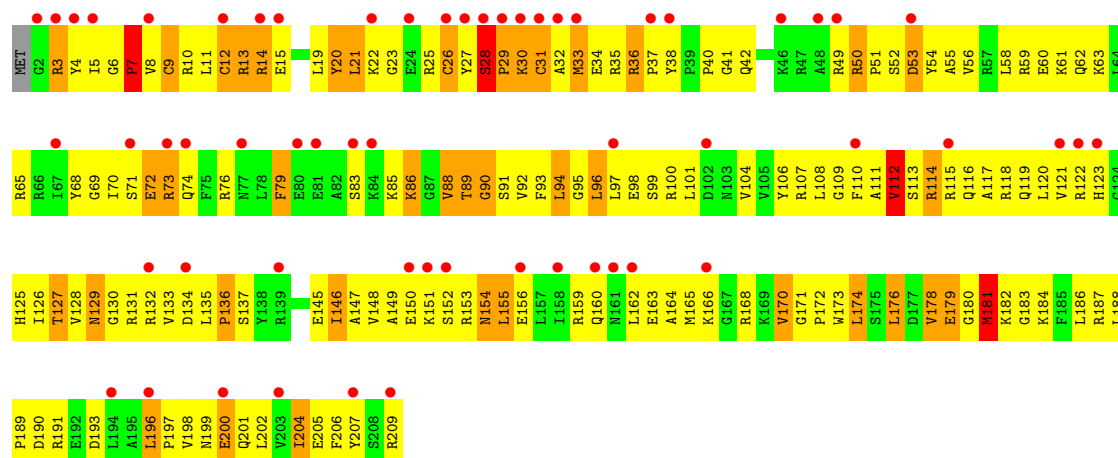




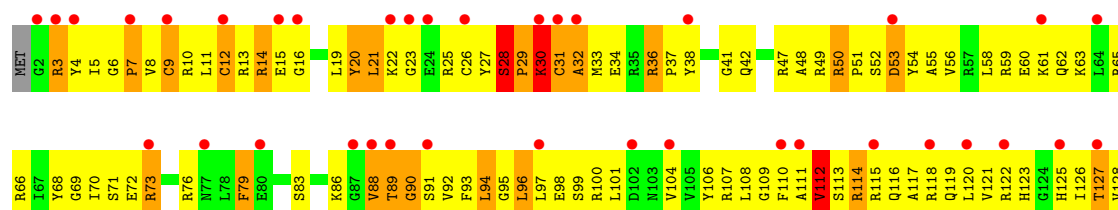
• Molecule 3: 30S ribosomal protein S3

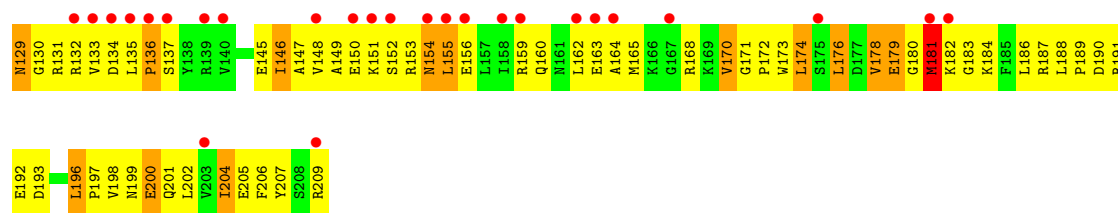


• Molecule 4: 30S ribosomal protein S4

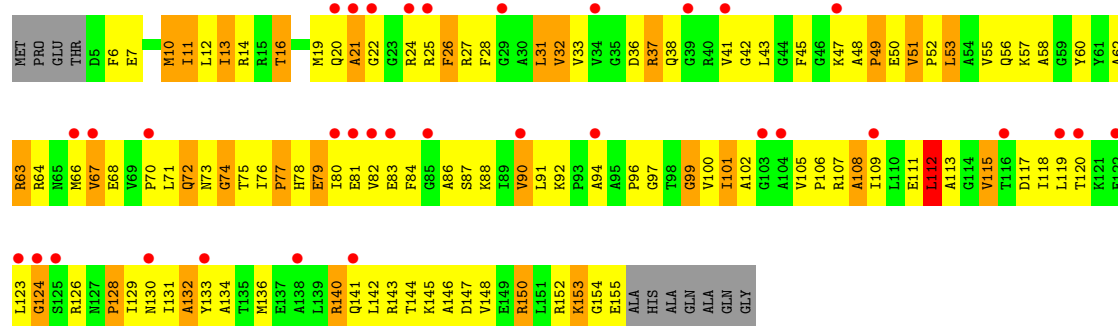


• Molecule 4: 30S ribosomal protein S4

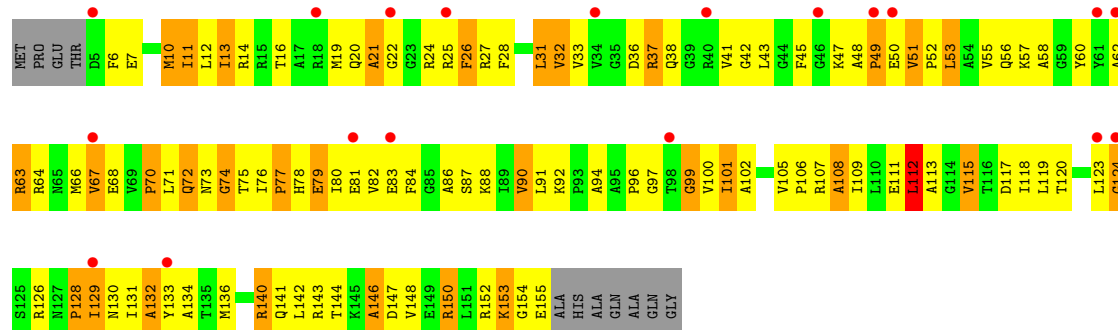




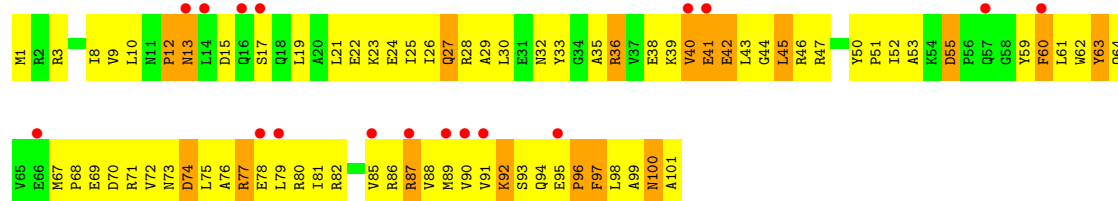
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

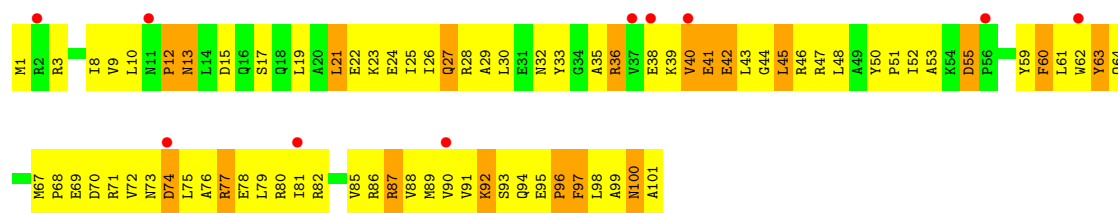


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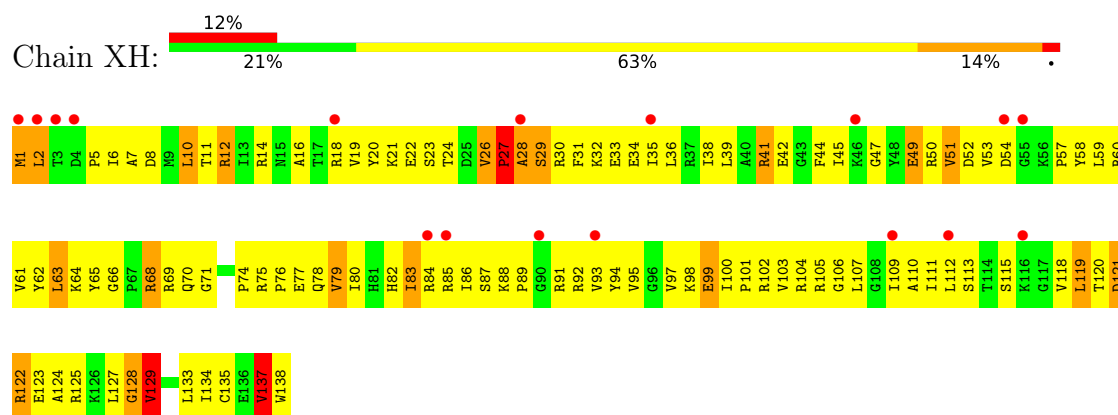


• Molecule 6: 30S ribosomal protein S6

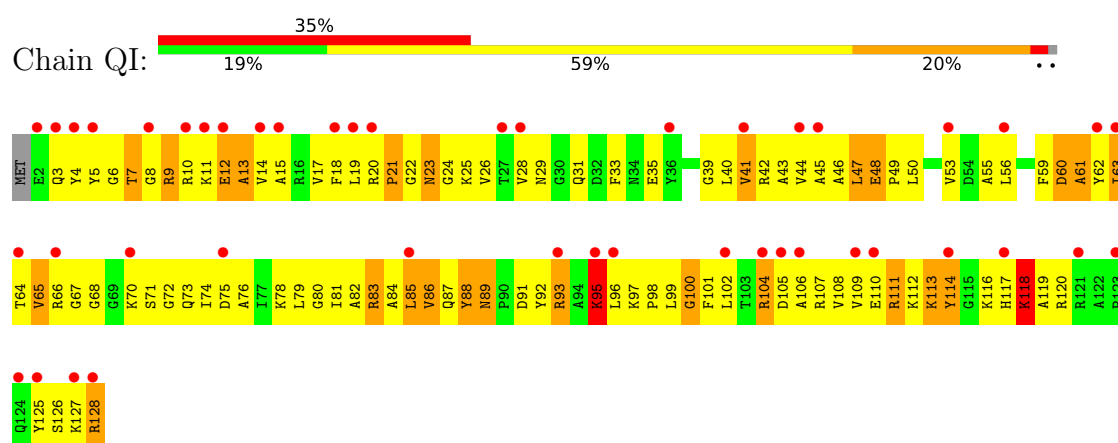




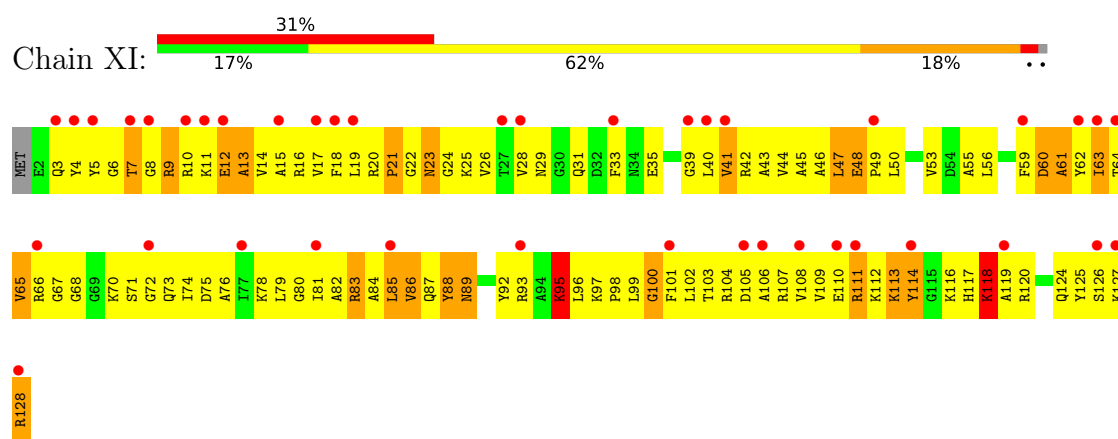
• Molecule 8: 30S ribosomal protein S8



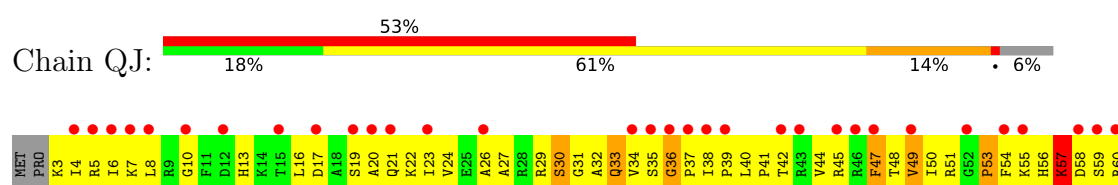
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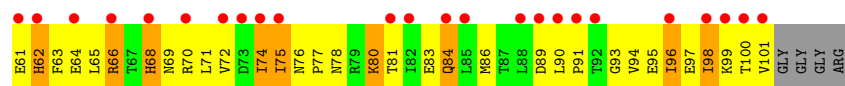


• Molecule 9: 30S ribosomal protein S9

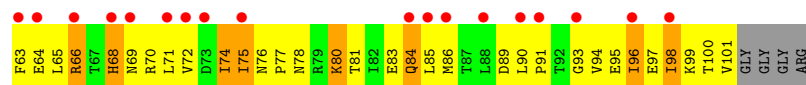
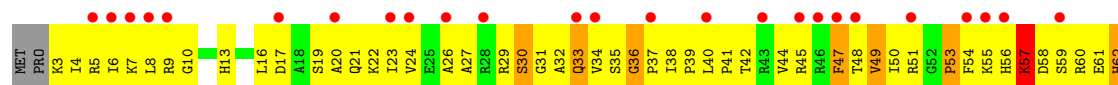


• Molecule 10: 30S ribosomal protein S10

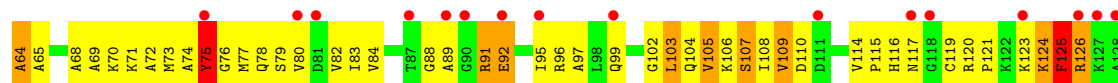
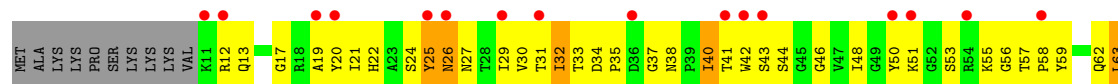




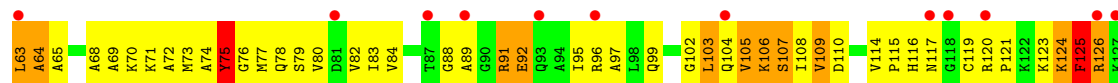
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

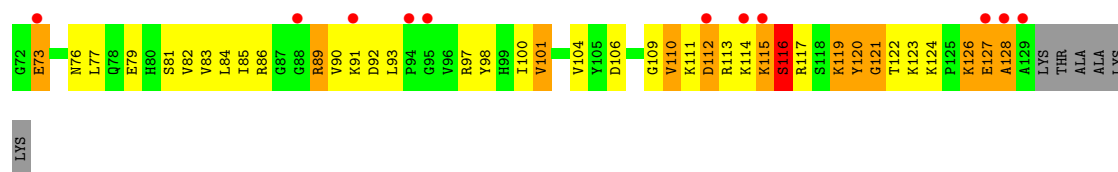


- Molecule 11: 30S ribosomal protein S11

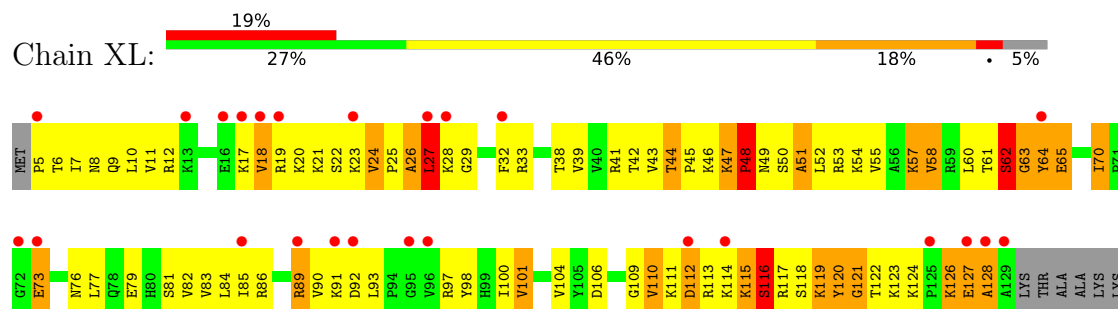


- Molecule 12: 30S ribosomal protein S12

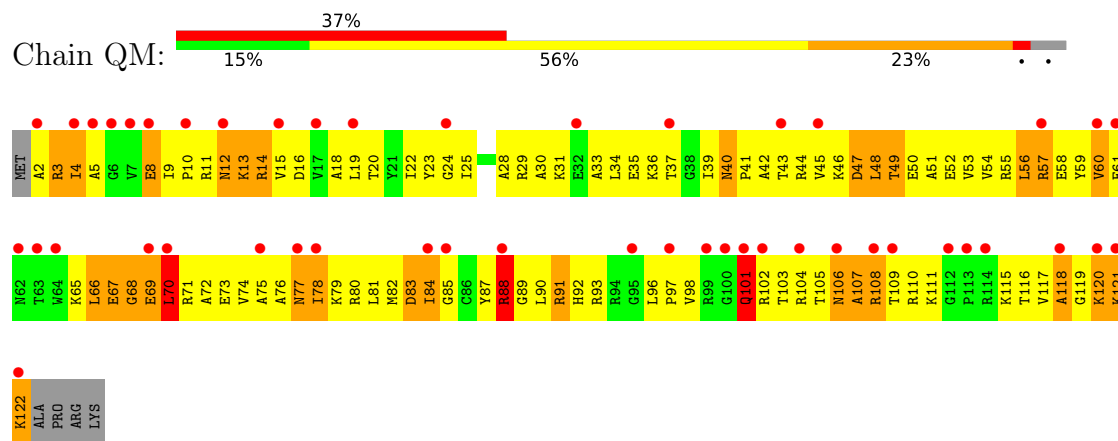




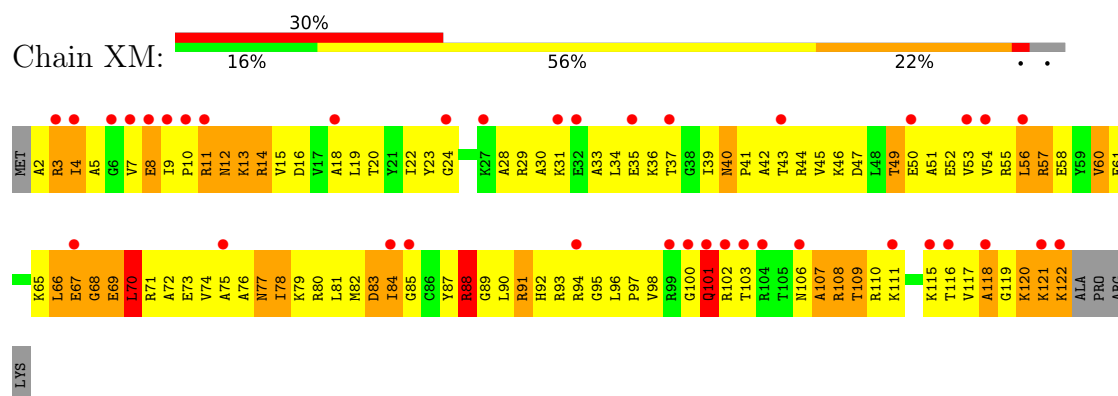
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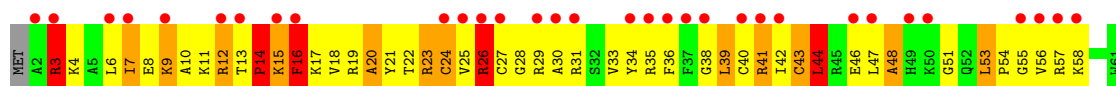
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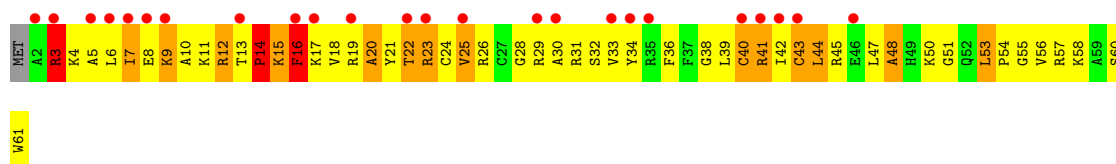
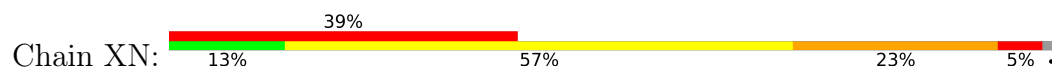
• Molecule 13: 30S ribosomal protein S13



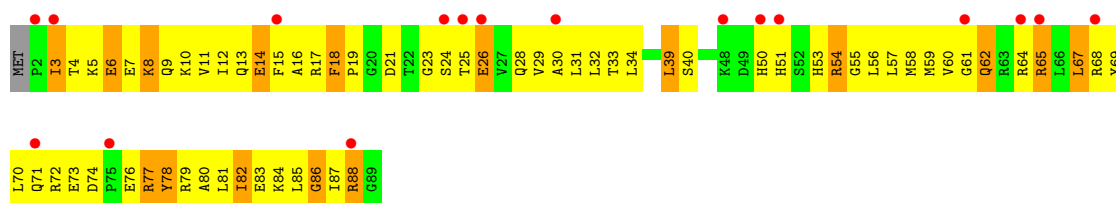
• Molecule 14: 30S ribosomal protein S14



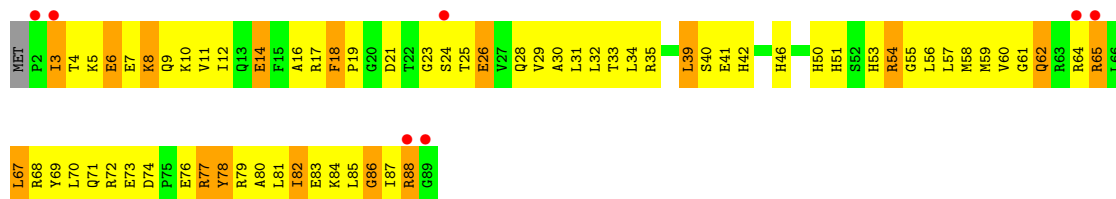
- Molecule 14: 30S ribosomal protein S14



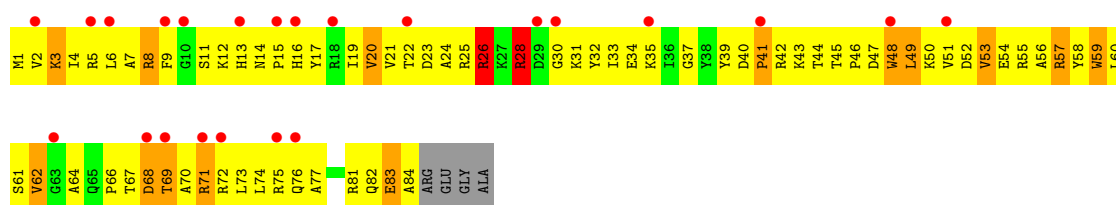
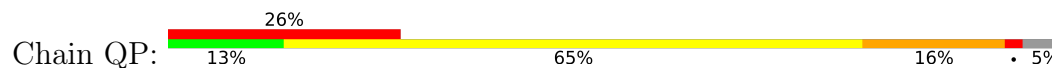
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

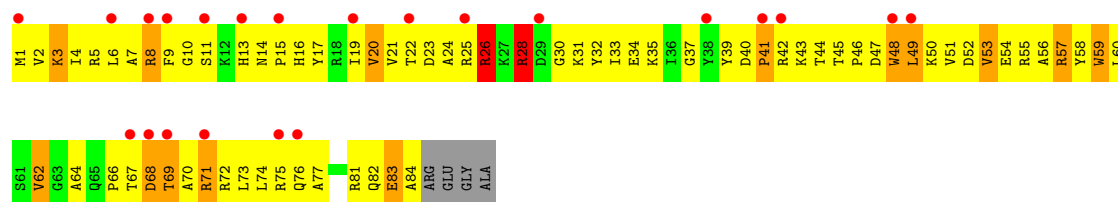


- Molecule 16: 30S ribosomal protein S16

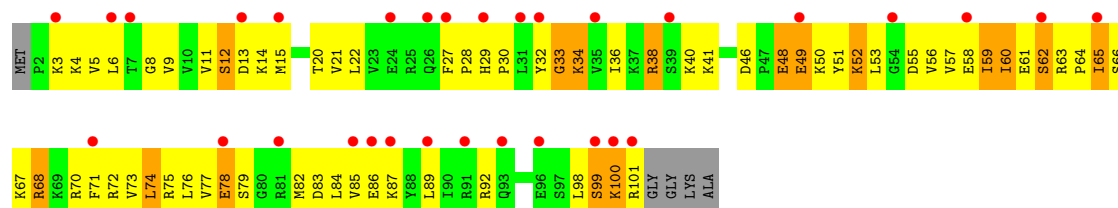


- Molecule 16: 30S ribosomal protein S16

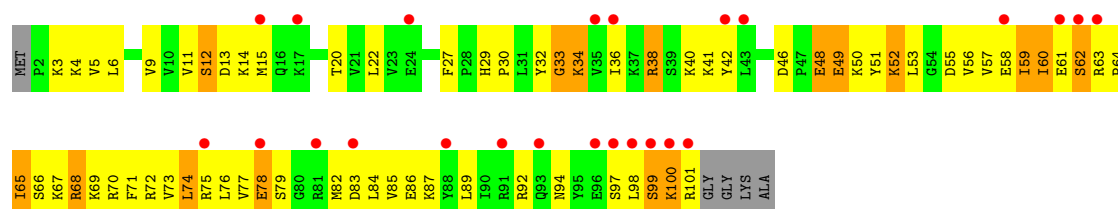




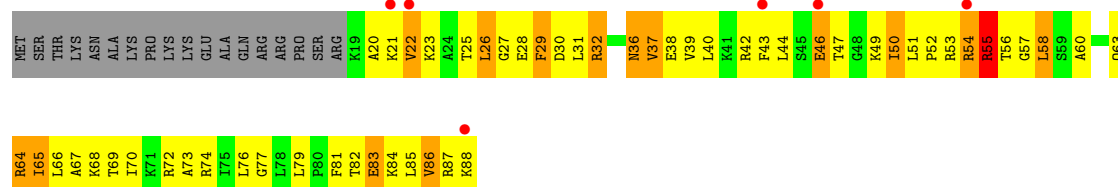
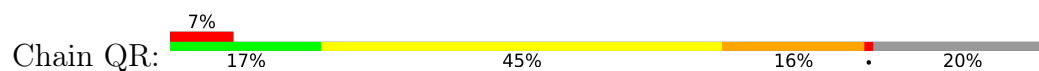
- Molecule 17: 30S ribosomal protein S17



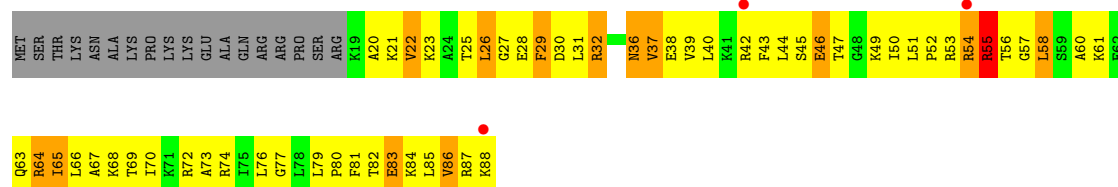
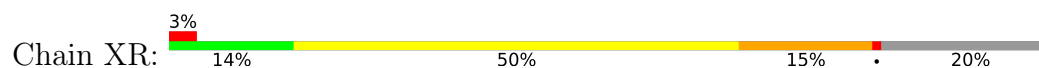
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

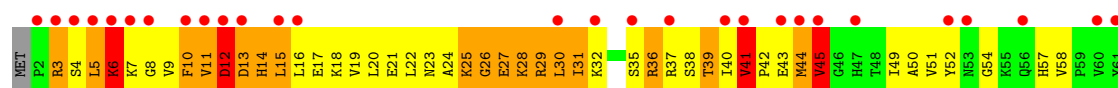
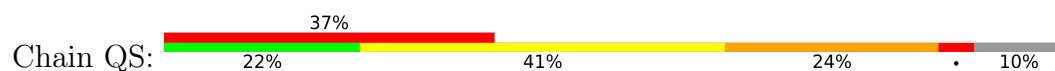


- Molecule 18: 30S ribosomal protein S18

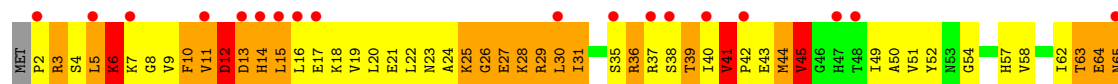
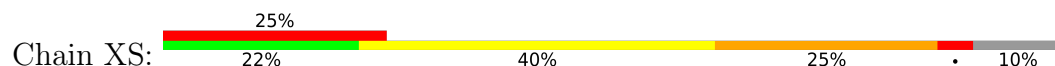




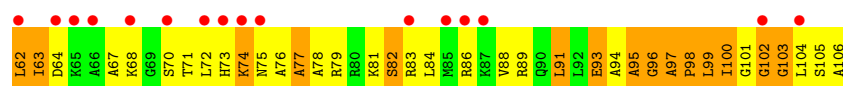
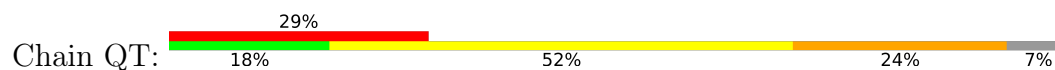
- Molecule 19: 30S ribosomal protein S19



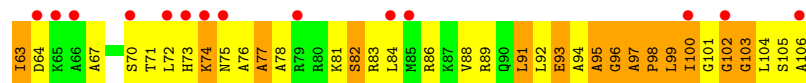
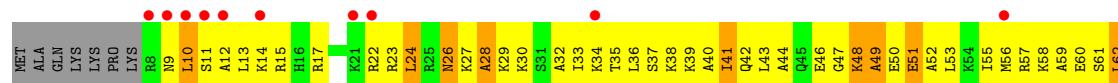
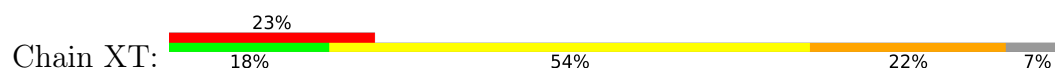
- Molecule 19: 30S ribosomal protein S19



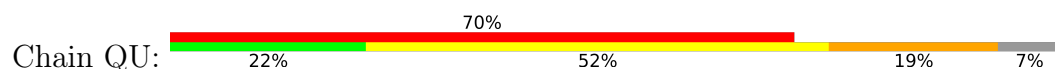
- Molecule 20: 30S ribosomal protein S20

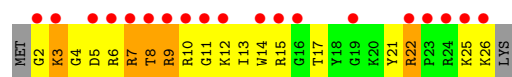


- Molecule 20: 30S ribosomal protein S20

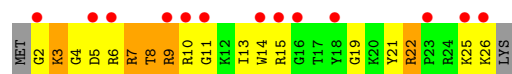


- Molecule 21: 30S ribosomal protein S21





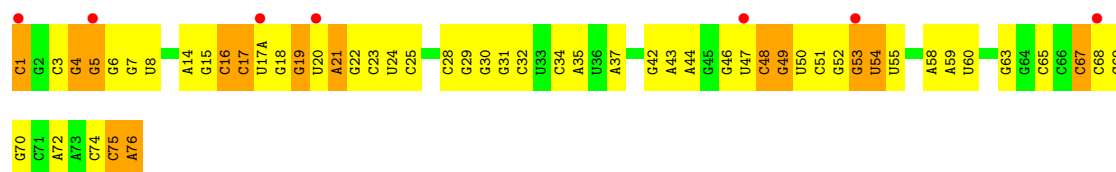
- Molecule 21: 30S ribosomal protein S21



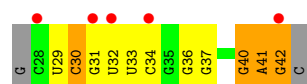
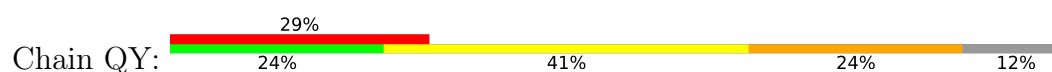
- Molecule 22: P-site tRNA fMet



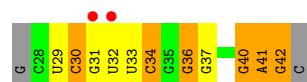
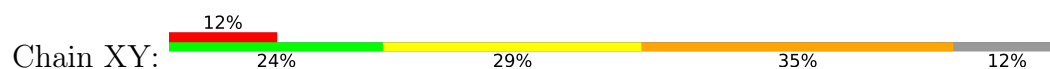
- Molecule 22: P-site tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



- Molecule 24: A-site ASL SufA6

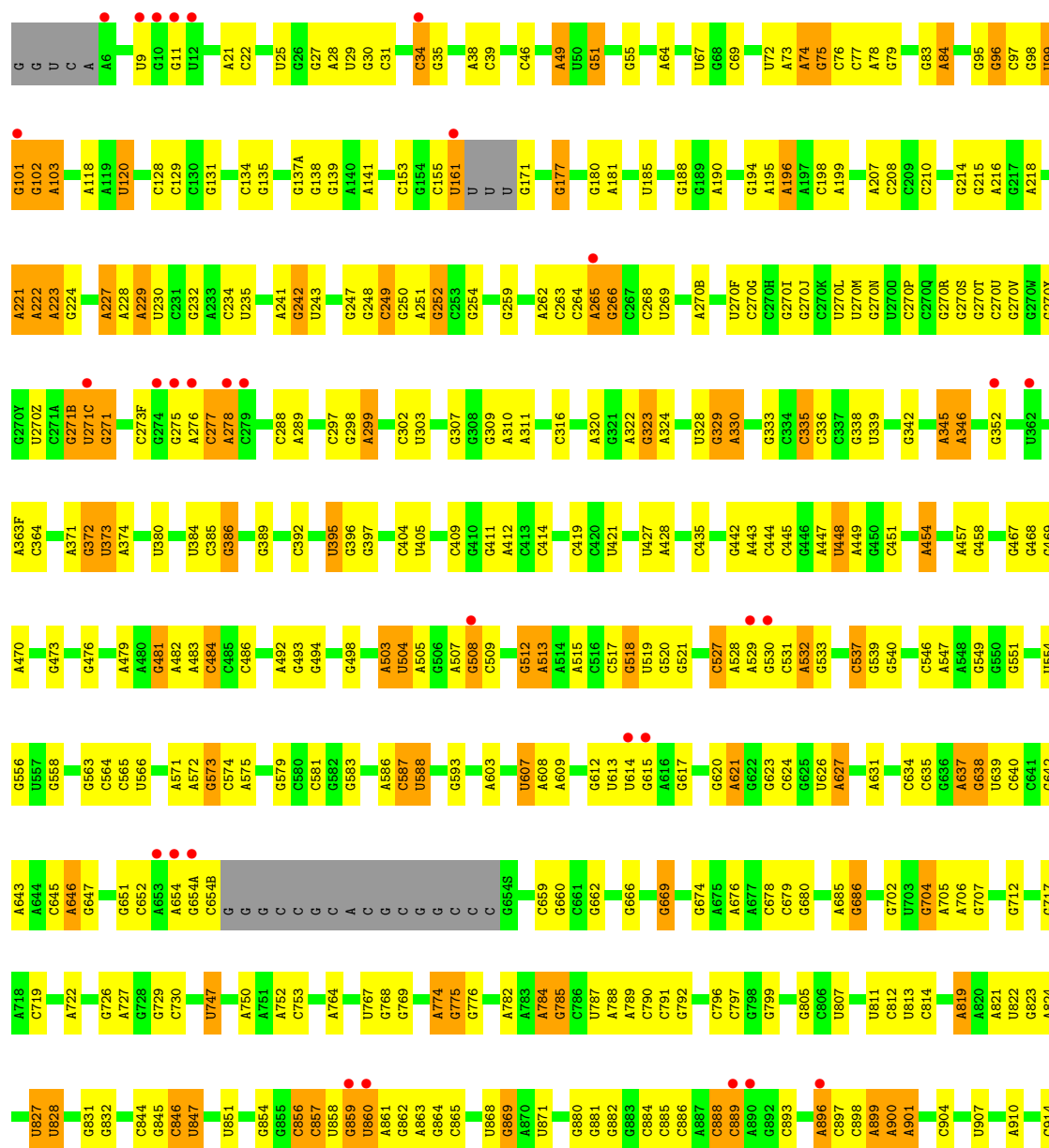




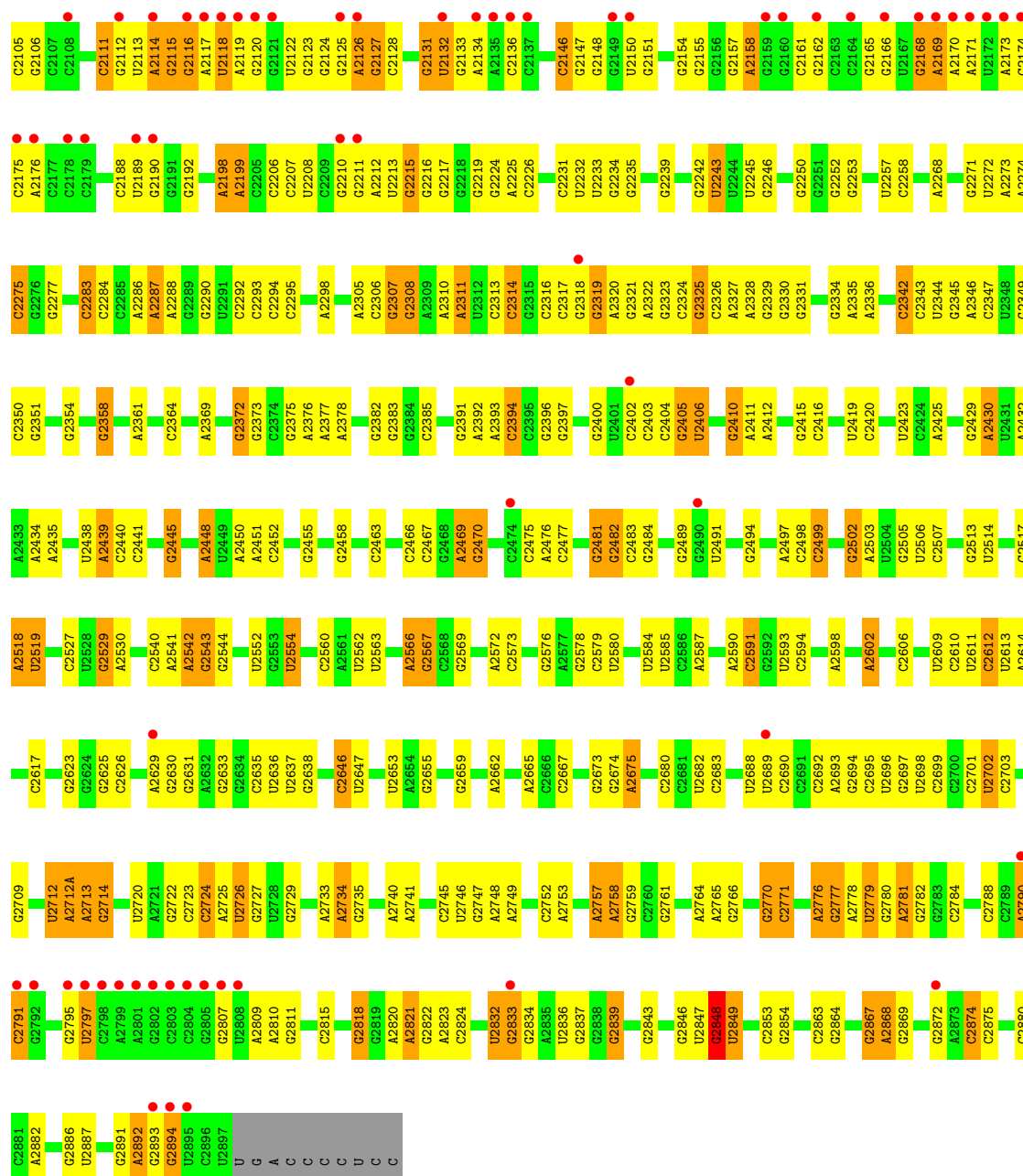
• Molecule 24: A-site ASL SufA6



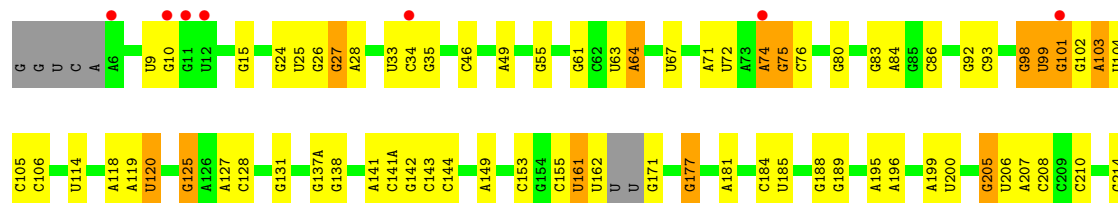
• Molecule 25: 23S rRNA

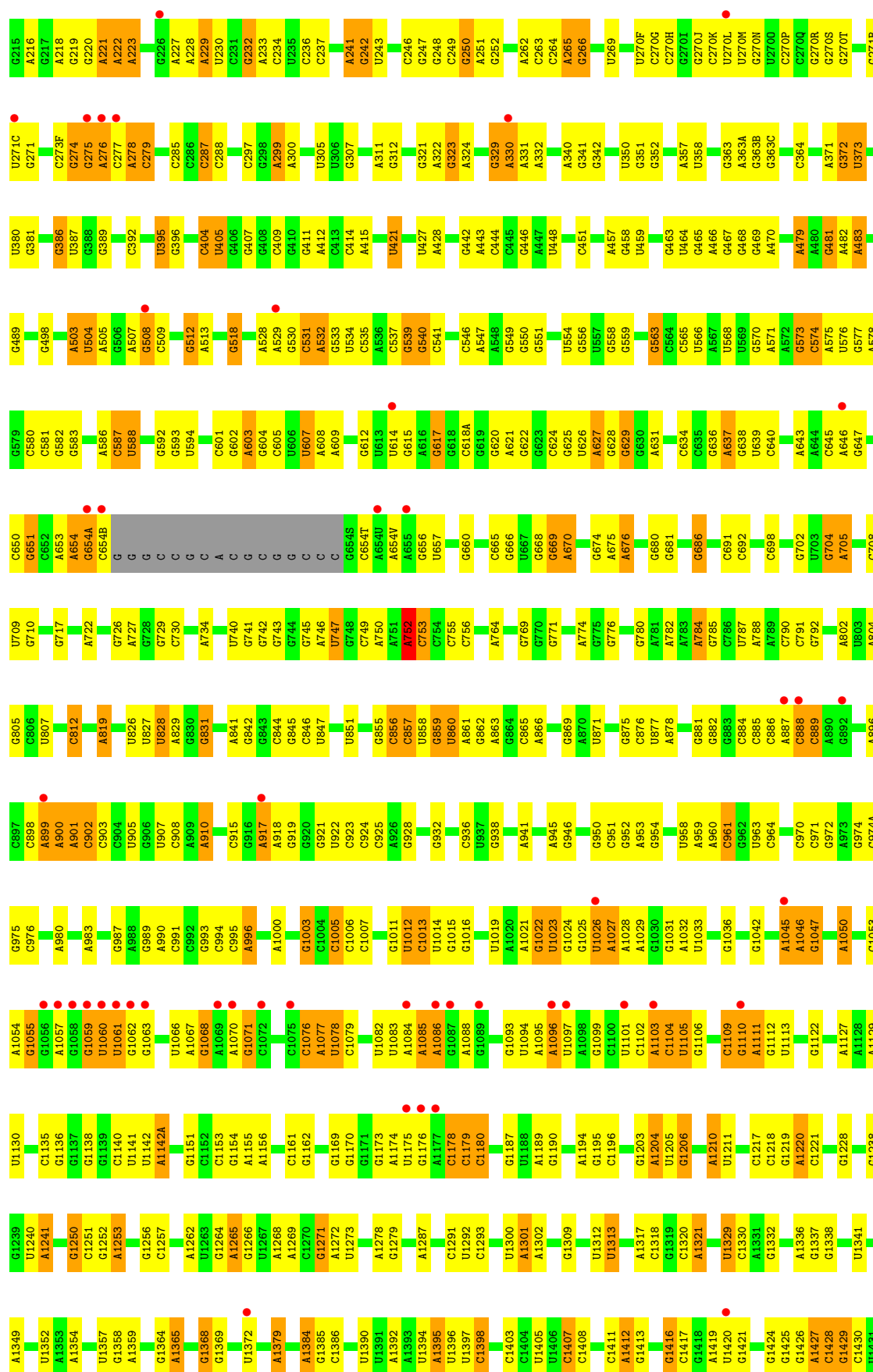


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| G2011 | C1905 | G1816 | C1589 | G1492 | C1411  | U1312 | A1210 | A1129 | U1065 | C998  | G9916  |
| G2012 | G1906 | G1817 | U1590 | C1493 | A1412  | U1313 | U1211 | U1130 | A1066 | C999  | A9917  |
| A2014 | A1913 | G1818 | G1591 | C1494 | A1413  | C1314 | G1216 | G1131 | A1067 | A1000 | C9923  |
| A2015 | A1918 | A1819 | C1592 | U1496 | G1416  | G1319 | C1217 | C1135 | G1068 | G1003 | C9924  |
| A2019 | A1919 | A1820 | G1593 | U1497 | G1417  | A1321 | A1220 | G1136 | A1069 | G1004 | C9925  |
| A2020 | C1920 | G1728 | C1594 | C1498 | A1419  | G1327 | G1224 | G1137 | A1070 | C1005 | G9926  |
| A2021 | G1826 | U1729 | C1595 | C1502 | A1417  | U1329 | A1227 | G1138 | G1071 | C1006 | A9928  |
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| G2070 | G1888 | C1795 | A1677 | A1567 | G1473  | A1386 | C1291 | C1188 | C1109 | A1048 | C9974A |
| A2071 | A1889 | U1796 | G1678 | G1568 | C1474  | G1386 | U1292 | C1189 | G1110 | C1049 | G9975  |
| G2072 | A1890 | C1797 | U1680 | A1569 | G1475  | U1391 | G1297 | G1190 | A1111 | A1050 | A9983  |
| C2073 | C1891 | U1798 | U1688 | C1577 | C1476  | U1394 | C1297 | G1195 | G1112 | A1054 | G987   |
| U2074 | C1892 | G1799 | A1689 | U1578 | A1477  | U1394 | U1300 | C1201 | G1115 | G1055 | A988   |
| U2075 | C1893 | C1800 | A1690 | A1579 | U1482  | A1395 | U1301 | C1202 | G1116 | G1056 | G989   |
| G2093 | C1894 | G1801 | C1694 | A1580 | G1483  | U1397 | A1301 | G1203 | G1117 | A1057 | A9990  |
| G2094 | G1895 | A1802 | G1695 | G1581 | G1484  | U1398 | C1304 | A1204 | G1058 | G1059 | C9991  |
| A2095 | G1896 | A1803 | A1698 | C1585 | G1485  | C1398 | C1305 | U1205 | G1122 | U1060 | C9992  |
| C2096 | G1899 | A1812 | A1699 | C1586 | A1486  | U1405 | C1306 | G1206 | G1125 | U1061 | G9993  |
| G2099 | C1902 | G1813 | A1701 | A1587 | G1487  | U1406 |       | C1208 | A1126 | G1062 | C9994  |
|       | G1903 | G1814 |       |       |        |       |       |       |       | G1063 | A9996  |

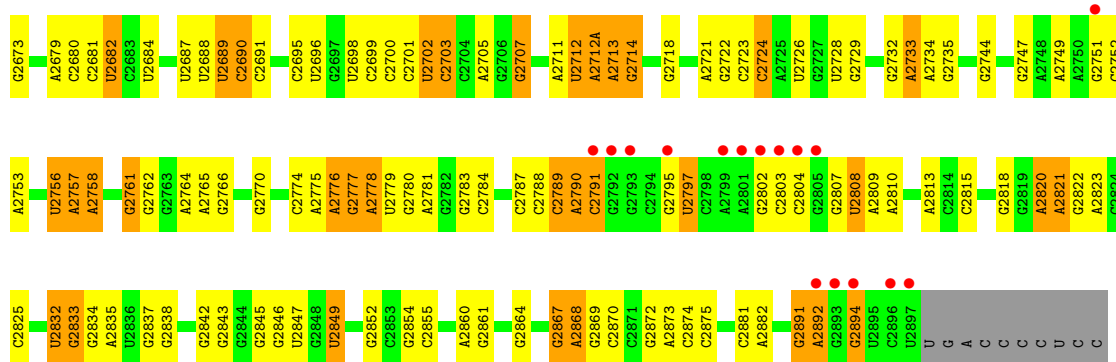


• Molecule 25: 23S rRNA

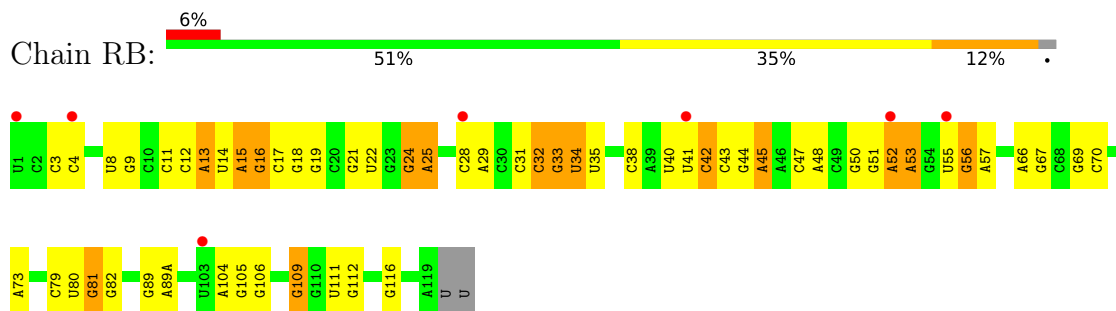




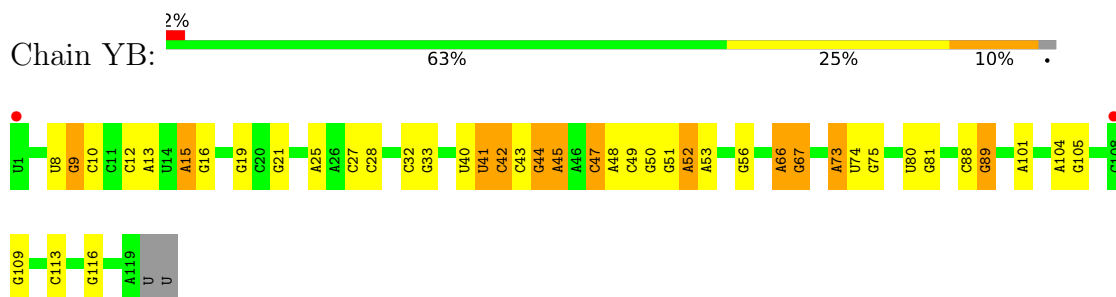
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| C2591 | C2489 | C2402 | C2318 | G2219 | A2134 | G2046 | C1957 | C1837 | C1742 | G1519 | C1432  |
| C2592 | G2490 | C2403 | G2319 | G2224 | A2135 | U2047 | C1958 | A1847 | G1743 | U1520 | U1433  |
| U2593 | G2491 | C2404 | G2320 | A2225 | C2137 | A2051 | G1959 | A1848 | G1750 | G1521 | A1434  |
| C2594 | G2494 | U2406 | A2321 | A2226 | G2138 | G2053 | U1963 | A1849 | G1755 | G1522 | G1441  |
|       |       |       | A2322 | A2227 | C2139 | G2054 | U1964 | A1850 | G1756 | G1523 | G1442  |
|       |       |       | G2323 |       | C2140 | A2055 | G1965 | G1858 | A1757 | G1530 | A1444A |
|       |       |       | G2324 |       | G2141 | G2056 | A1966 | A1859 | G1758 | C1533 | C1445  |
|       |       |       | G2325 |       | G2142 | C2057 | G1967 | G1862 | G1759 | C1534 |        |
|       |       |       | G2326 |       | G2143 | G2058 | G1968 | G1863 | A1760 | U1535 | A1449  |
|       |       |       | G2327 |       | U2150 | A2059 | G1969 | U1864 | G1761 | U1536 | G1449A |
|       |       |       | G2328 |       | G2151 | A2060 | A1970 | G1865 | G1762 | C1537 | U1454  |
|       |       |       | A2329 |       | G2152 | G2061 | A1971 | G1866 | G1763 | G1538 | G1455  |
|       |       |       | G2330 |       | G2153 | A2062 | A1972 | A1870 | G1764 | U1539 | C1458  |
|       |       |       | G2331 |       | G2154 | C2063 | G1973 | A1871 | G1765 | U1540 | G1459  |
|       |       |       |       |       | G2155 |       |       | A1872 | G1766 | A1460 | A1461  |
|       |       |       |       |       | G2156 |       |       | A1873 | G1767 | C1544 | C1467  |
|       |       |       |       |       | G2157 |       |       | A1874 | G1768 | A1545 |        |
|       |       |       |       |       | G2158 |       |       | A1875 | G1769 | C1549 | A1471  |
|       |       |       |       |       | G2159 |       |       | A1876 | G1770 | A1472 | A1473  |
|       |       |       |       |       | G2160 |       |       | A1877 | G1771 | A1558 | A1474  |
|       |       |       |       |       | G2161 |       |       | A1878 | G1772 | G1559 |        |
|       |       |       |       |       | G2162 |       |       | A1879 | G1773 | A1566 | G1478  |
|       |       |       |       |       | G2163 |       |       | A1880 | G1774 | A1569 | G1479  |
|       |       |       |       |       | G2164 |       |       | A1881 | G1775 | G1480 | G1481  |
|       |       |       |       |       | G2165 |       |       | A1882 | G1776 | U1482 | G1483  |
|       |       |       |       |       | G2166 |       |       | A1883 | G1777 | G1484 | G1485  |
|       |       |       |       |       | G2167 |       |       | A1884 | G1778 | A1581 | A1490  |
|       |       |       |       |       | G2168 |       |       | A1885 | G1779 | C1582 | A1491  |
|       |       |       |       |       | G2169 |       |       | A1886 | G1780 | A1583 | G1492  |
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|       |       |       |       |       | G2172 |       |       | A1889 | G1783 | G1594 | U1497  |
|       |       |       |       |       | G2173 |       |       | A1890 | G1784 | G1595 | G1500  |
|       |       |       |       |       | G2174 |       |       | A1891 | G1785 | C1598 | C1505  |
|       |       |       |       |       | G2175 |       |       | A1892 | G1786 | G1605 | A1507  |
|       |       |       |       |       | G2176 |       |       | A1893 | G1787 | G1606 | A1508  |
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|       |       |       |       |       | G2178 |       |       | A1895 | G1789 | A1608 | A1510  |
|       |       |       |       |       | G2179 |       |       | A1896 | G1790 | A1511 | G1512  |
|       |       |       |       |       | G2180 |       |       | A1897 | G1791 | A1513 | C1513  |
|       |       |       |       |       | G2181 |       |       | A1898 | G1792 | C1514 | U1514  |
|       |       |       |       |       | G2182 |       |       | A1899 | G1793 | A1617 | C1515  |
|       |       |       |       |       | G2183 |       |       | A1900 | G1794 | A1618 | U1516  |
|       |       |       |       |       | G2184 |       |       | A1901 | G1795 | C1636 | C1518  |
|       |       |       |       |       | G2185 |       |       | A1902 | G1796 |       |        |
|       |       |       |       |       | G2186 |       |       | A1903 | G1797 |       |        |
|       |       |       |       |       | G2187 |       |       | A1904 | G1798 |       |        |
|       |       |       |       |       | G2188 |       |       | A1905 | G1799 |       |        |
|       |       |       |       |       | G2189 |       |       | A1906 | G1800 |       |        |
|       |       |       |       |       | G2190 |       |       | A1907 | G1801 |       |        |
|       |       |       |       |       | G2191 |       |       | A1908 | G1802 |       |        |
|       |       |       |       |       | G2192 |       |       | A1909 | G1803 |       |        |
|       |       |       |       |       | G2193 |       |       | A1910 | G1804 |       |        |
|       |       |       |       |       | G2194 |       |       | A1911 | G1805 |       |        |
|       |       |       |       |       | G2195 |       |       | A1912 | G1806 |       |        |
|       |       |       |       |       | G2196 |       |       | A1913 | G1807 |       |        |
|       |       |       |       |       | G2197 |       |       | A1914 | G1808 |       |        |
|       |       |       |       |       | G2198 |       |       | A1915 | G1809 |       |        |
|       |       |       |       |       | G2199 |       |       | A1916 | G1810 |       |        |
|       |       |       |       |       | G2200 |       |       | A1917 | G1811 |       |        |
|       |       |       |       |       | G2201 |       |       | A1918 | G1812 |       |        |
|       |       |       |       |       | G2202 |       |       | A1919 | G1813 |       |        |
|       |       |       |       |       | G2203 |       |       | A1920 | G1814 |       |        |
|       |       |       |       |       | G2204 |       |       | A1921 | G1815 |       |        |
|       |       |       |       |       | G2205 |       |       | A1922 | G1816 |       |        |
|       |       |       |       |       | G2206 |       |       | A1923 | G1817 |       |        |
|       |       |       |       |       | G2207 |       |       | A1924 | G1818 |       |        |
|       |       |       |       |       | G2208 |       |       | A1925 | G1819 |       |        |
|       |       |       |       |       | G2209 |       |       | A1926 | G1820 |       |        |
|       |       |       |       |       | G2210 |       |       | A1927 | G1821 |       |        |
|       |       |       |       |       | G2211 |       |       | A1928 | G1822 |       |        |
|       |       |       |       |       | G2212 |       |       | A1929 | G1823 |       |        |
|       |       |       |       |       | G2213 |       |       | A1930 | G1824 |       |        |
|       |       |       |       |       | G2214 |       |       | A1931 | G1825 |       |        |
|       |       |       |       |       | G2215 |       |       | A1932 | G1826 |       |        |
|       |       |       |       |       | G2216 |       |       | A1933 | G1827 |       |        |
|       |       |       |       |       | G2217 |       |       | A1934 | G1828 |       |        |
|       |       |       |       |       | G2218 |       |       | A1935 | G1829 |       |        |
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|       |       |       |       |       | G2220 |       |       | A1937 | G1831 |       |        |
|       |       |       |       |       | G2221 |       |       | A1938 | G1832 |       |        |
|       |       |       |       |       | G2222 |       |       | A1939 | G1833 |       |        |
|       |       |       |       |       | G2223 |       |       | A1940 | G1834 |       |        |
|       |       |       |       |       | G2224 |       |       | A1941 | G1835 |       |        |
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|       |       |       |       |       | G2226 |       |       | A1943 | G1837 |       |        |
|       |       |       |       |       | G2227 |       |       | A1944 | G1838 |       |        |
|       |       |       |       |       | G2228 |       |       | A1945 | G1839 |       |        |
|       |       |       |       |       | G2229 |       |       | A1946 | G1840 |       |        |
|       |       |       |       |       | G2230 |       |       | A1947 | G1841 |       |        |
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|       |       |       |       |       | G2232 |       |       | A1949 | G1843 |       |        |
|       |       |       |       |       | G2233 |       |       | A1950 | G1844 |       |        |
|       |       |       |       |       | G2234 |       |       | A1951 | G1845 |       |        |
|       |       |       |       |       | G2235 |       |       | A1952 | G1846 |       |        |
|       |       |       |       |       | G2236 |       |       | A1953 | G1847 |       |        |
|       |       |       |       |       | G2237 |       |       | A1954 | G1848 |       |        |
|       |       |       |       |       | G2238 |       |       | A1955 | G1849 |       |        |
|       |       |       |       |       | G2239 |       |       | A1956 | G1850 |       |        |
|       |       |       |       |       | G2240 |       |       | A1957 | G1851 |       |        |
|       |       |       |       |       | G2241 |       |       | A1958 | G1852 |       |        |
|       |       |       |       |       | G2242 |       |       | A1959 | G1853 |       |        |
|       |       |       |       |       | G2243 |       |       | A1960 | G1854 |       |        |
|       |       |       |       |       | G2244 |       |       | A1961 | G1855 |       |        |
|       |       |       |       |       | G2245 |       |       | A1962 | G1856 |       |        |
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|       |       |       |       |       | G2253 |       |       | A1970 | G1864 |       |        |
|       |       |       |       |       | G2254 |       |       | A1971 | G1865 |       |        |
|       |       |       |       |       | G2255 |       |       | A1972 | G1866 |       |        |
|       |       |       |       |       | G2256 |       |       | A1973 | G1867 |       |        |
|       |       |       |       |       | G2257 |       |       | A1974 | G1868 |       |        |
|       |       |       |       |       | G2258 |       |       | A1975 | G1869 |       |        |
|       |       |       |       |       | G2259 |       |       | A1976 | G1870 |       |        |
|       |       |       |       |       | G2260 |       |       | A1977 | G1871 |       |        |
|       |       |       |       |       | G2261 |       |       | A1978 | G1872 |       |        |
|       |       |       |       |       | G2262 |       |       | A1979 | G1873 |       |        |
|       |       |       |       |       | G2263 |       |       | A1980 | G1874 |       |        |
|       |       |       |       |       | G2264 |       |       | A1981 | G1875 |       |        |
|       |       |       |       |       | G2265 |       |       | A1982 | G1876 |       |        |
|       |       |       |       |       | G2266 |       |       | A1983 | G1877 |       |        |
|       |       |       |       |       | G2267 |       |       | A1984 | G1878 |       |        |
|       |       |       |       |       | G2268 |       |       | A1985 | G1879 |       |        |
|       |       |       |       |       | G2269 |       |       | A1986 | G1880 |       |        |
|       |       |       |       |       | G2270 |       |       | A1987 | G1881 |       |        |
|       |       |       |       |       | G2271 |       |       | A1988 | G1882 |       |        |
|       |       |       |       |       | G2272 |       |       | A1989 | G1883 |       |        |
|       |       |       |       |       | G2273 |       |       | A1990 | G1884 |       |        |
|       |       |       |       |       | G2274 |       |       | A1991 | G1885 |       |        |
|       |       |       |       |       | G2275 |       |       | A1992 | G1886 |       |        |
|       |       |       |       |       | G2276 |       |       | A1993 | G1887 |       |        |
|       |       |       |       |       | G2277 |       |       | A1994 | G1888 |       |        |
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|       |       |       |       |       | G2282 |       |       | A1999 | G1893 |       |        |
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|       |       |       |       |       | G2284 |       |       | A2001 | G1895 |       |        |
|       |       |       |       |       | G2285 |       |       | A2002 | G1896 |       |        |
|       |       |       |       |       | G2286 |       |       | A2003 | G1897 |       |        |
|       |       |       |       |       | G2287 |       |       | A2004 | G1898 |       |        |
|       |       |       |       |       | G2288 |       |       | A2005 | G1899 |       |        |
|       |       |       |       |       | G2289 |       |       | A2006 | G1900 |       |        |
|       |       |       |       |       | G2290 |       |       | A2007 | G1901 |       |        |
|       |       |       |       |       | G2291 |       |       | A2008 | G1902 |       |        |
|       |       |       |       |       | G2292 |       |       | A2009 | G1903 |       |        |
|       |       |       |       |       | G2293 |       |       | A2010 | G1904 |       |        |
|       |       |       |       |       | G2294 |       |       | A2011 | G1905 |       |        |
|       |       |       |       |       | G2295 |       |       | A2012 | G1906 |       |        |
|       |       |       |       |       | G2296 |       |       | A2013 | G1907 |       |        |
|       |       |       |       |       | G2297 |       |       | A2014 | G1908 |       |        |
|       |       |       |       |       | G2298 |       |       | A2015 | G1909 |       |        |
|       |       |       |       |       | G2299 |       |       | A2016 | G1910 |       |        |
|       |       |       |       |       | G2300 |       |       | A2017 | G1911 |       |        |
|       |       |       |       |       | G2301 |       |       | A2018 | G1912 |       |        |
|       |       |       |       |       | G2302 |       |       | A2019 | G1913 |       |        |
|       |       |       |       |       | G2303 |       |       | A2020 | G1914 |       |        |
|       |       |       |       |       | G2304 |       |       | A2021 | G1915 |       |        |
|       |       |       |       |       | G2305 |       |       | A2022 | G1916 |       |        |
|       |       |       |       |       | G2306 |       |       | A2023 | G1917 |       |        |
|       |       |       |       |       | G2307 |       |       | A2024 | G1918 |       |        |
|       |       |       |       |       | G2308 |       |       | A2025 | G1919 |       |        |
|       |       |       |       |       | G2309 |       |       | A2026 | G1920 |       |        |
|       |       |       |       |       | G2310 |       |       | A2027 | G1921 |       |        |
|       |       |       |       |       | G2311 |       |       | A2028 | G1922 |       |        |
|       |       |       |       |       | G2312 |       |       | A2029 | G1923 | </    |        |



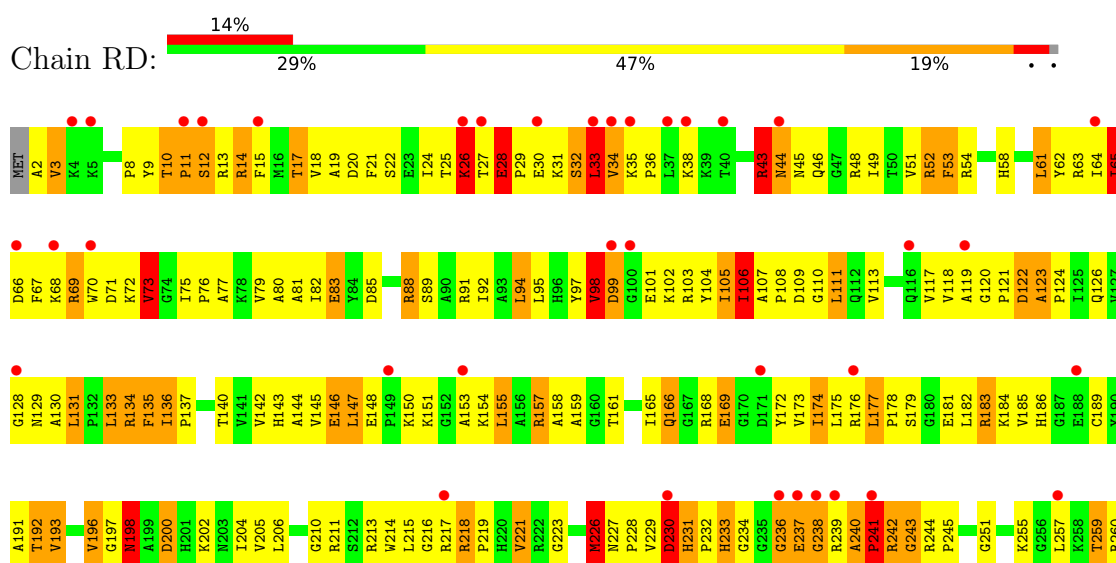
• Molecule 26: 5S rRNA



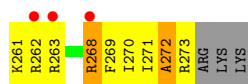
• Molecule 26: 5S rRNA



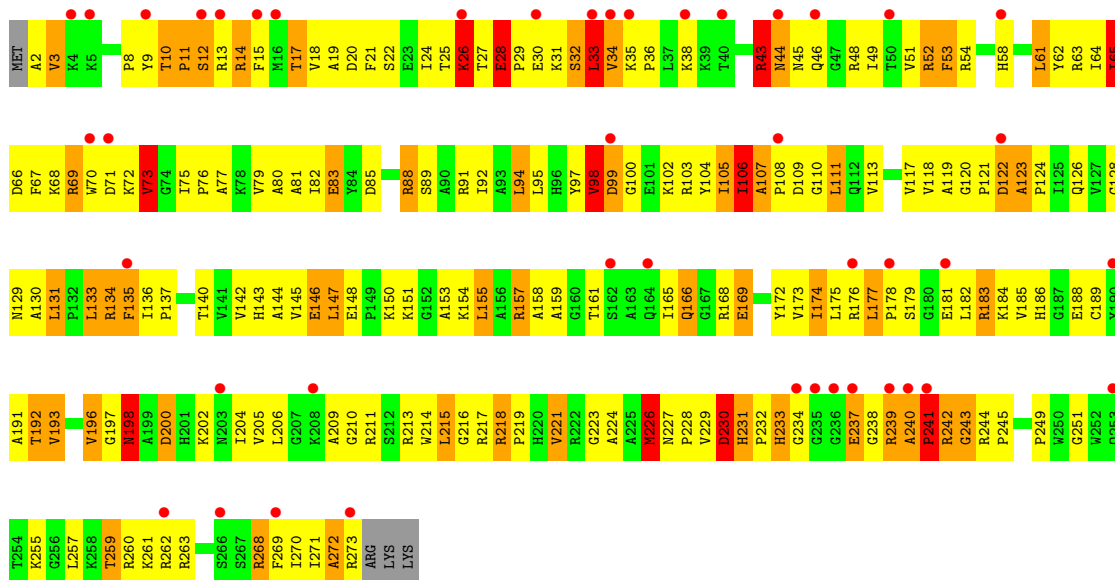
• Molecule 27: 50S ribosomal protein L2



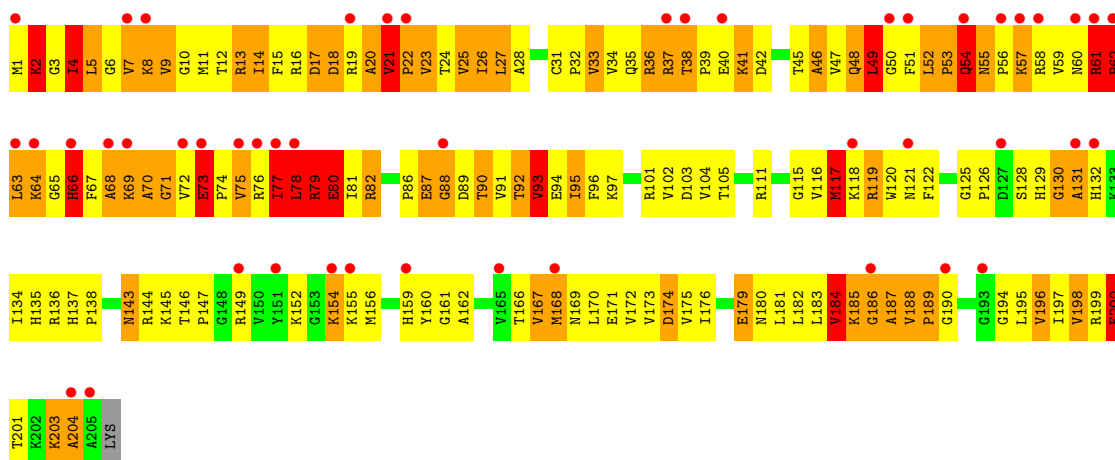
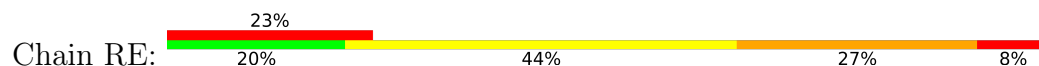




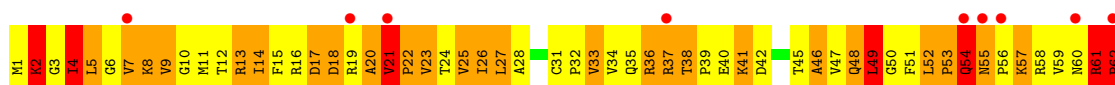
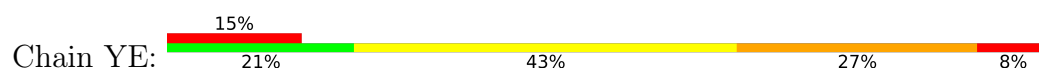
• Molecule 27: 50S ribosomal protein L2

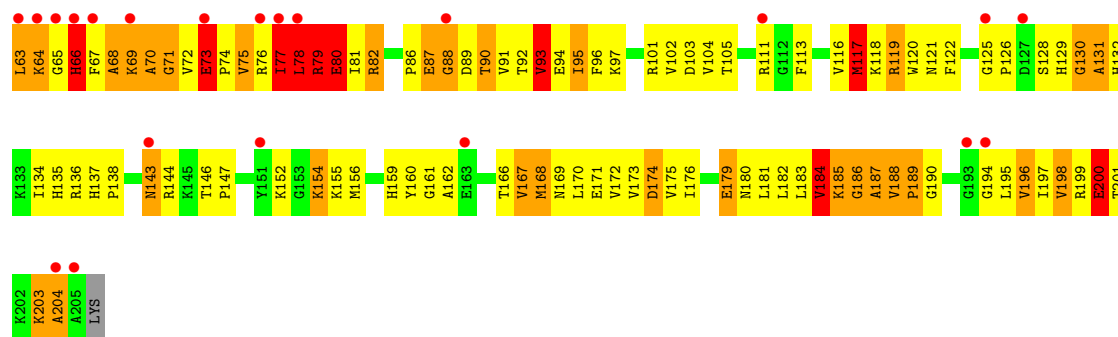


• Molecule 28: 50S ribosomal protein L3

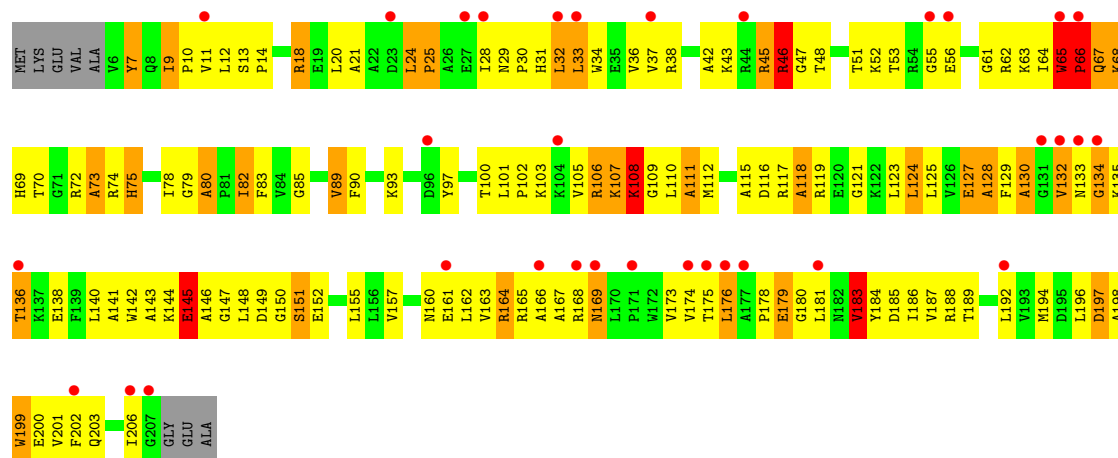


• Molecule 28: 50S ribosomal protein L3

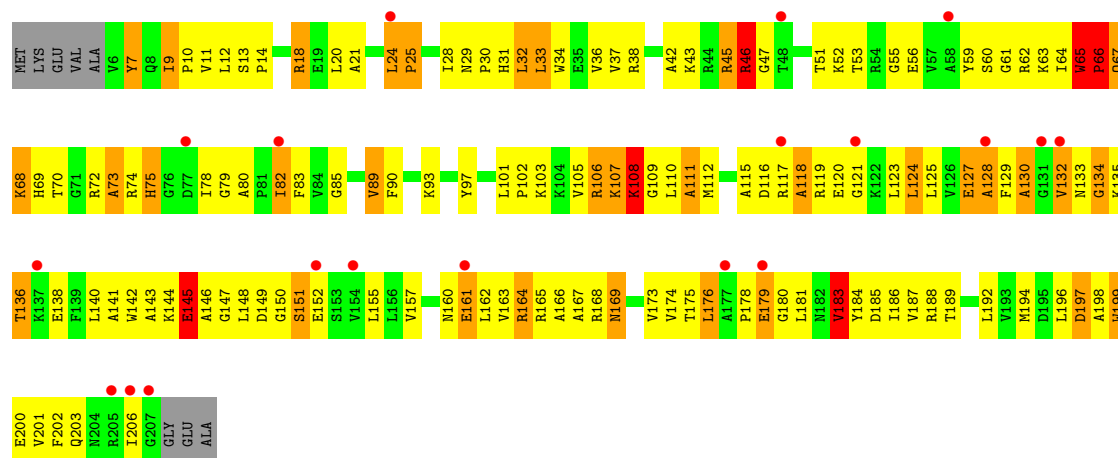




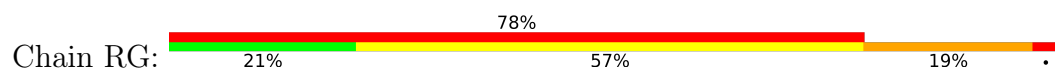
• Molecule 29: 50S ribosomal protein L4

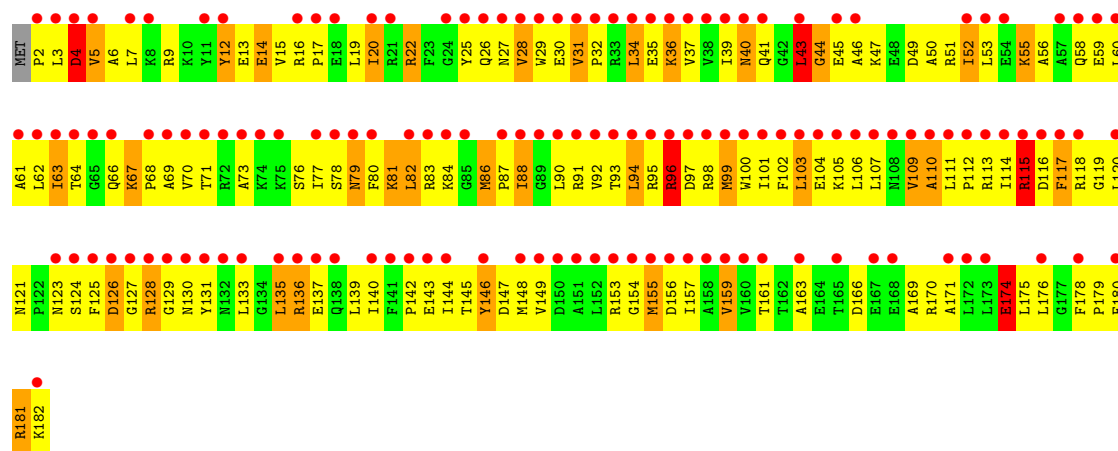


• Molecule 29: 50S ribosomal protein L4



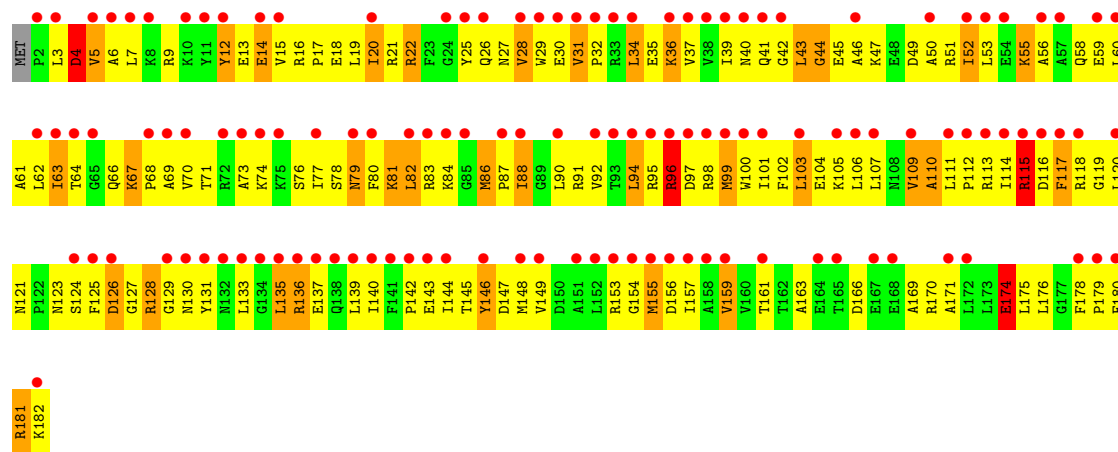
• Molecule 30: 50S ribosomal protein L5





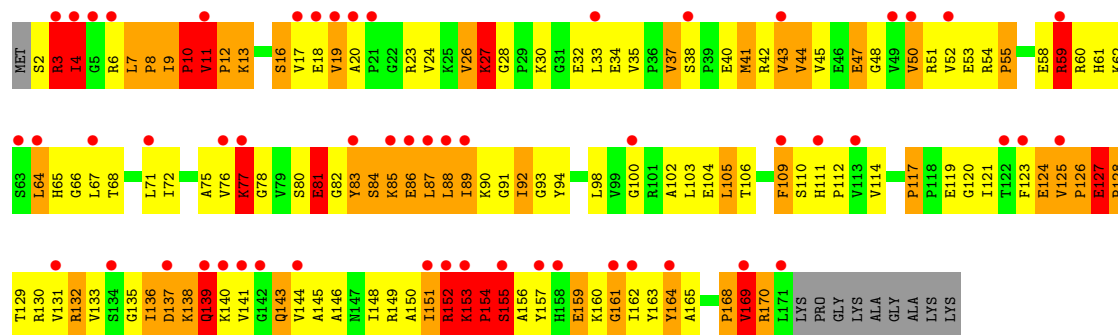
• Molecule 30: 50S ribosomal protein L5

Chain YG: 20% 69% 59% 19% ..



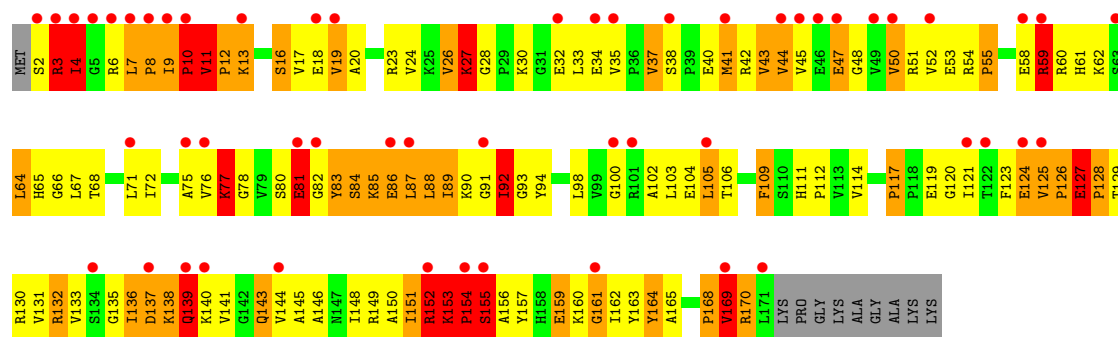
• Molecule 31: 50S ribosomal protein L6

Chain RH: 22% 31% 41% 23% 8% 6%

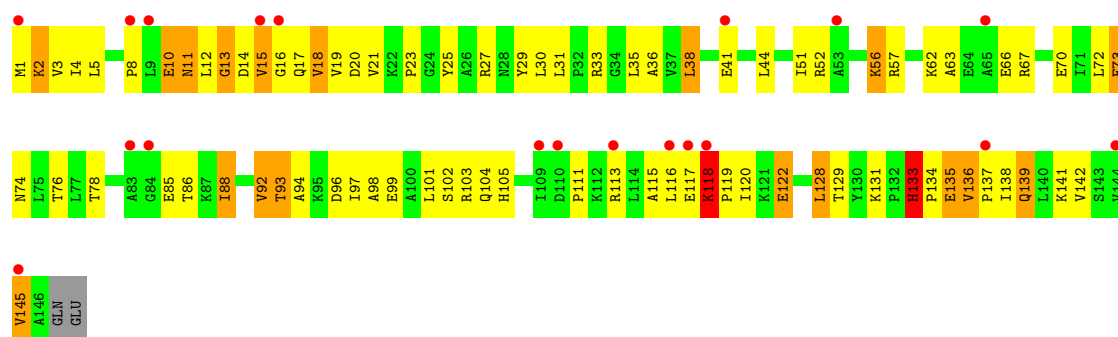
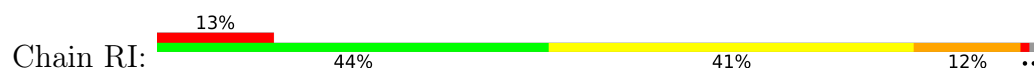


• Molecule 31: 50S ribosomal protein L6

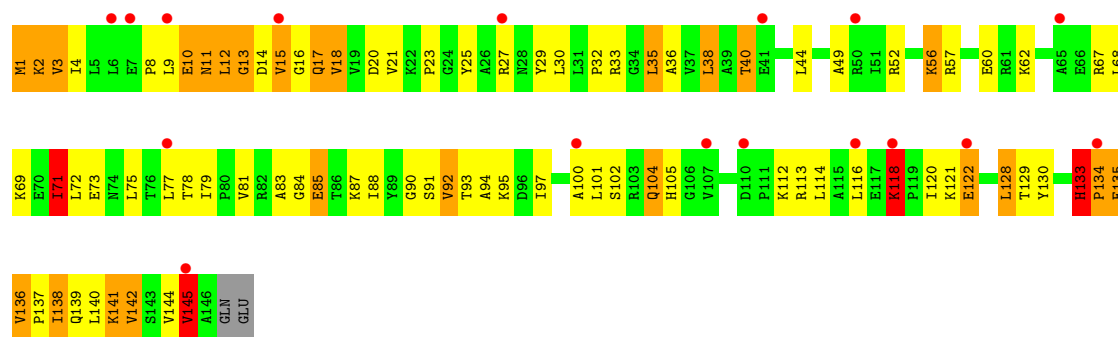
Chain YH: 22% 29% 41% 23% 9% 6%



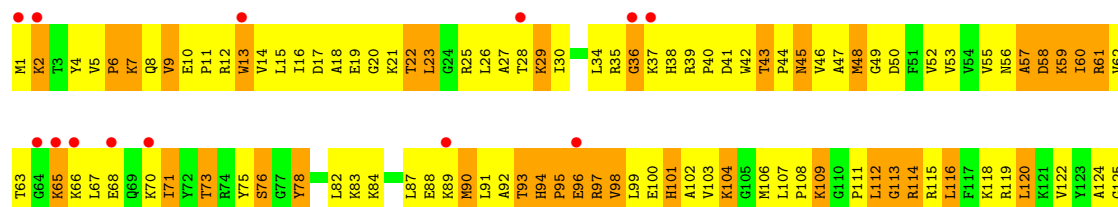
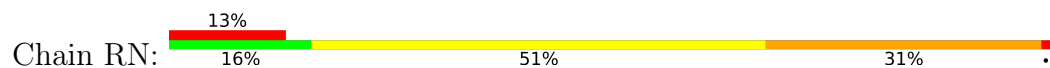
• Molecule 32: 50S ribosomal protein L9

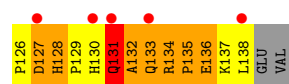


• Molecule 32: 50S ribosomal protein L9

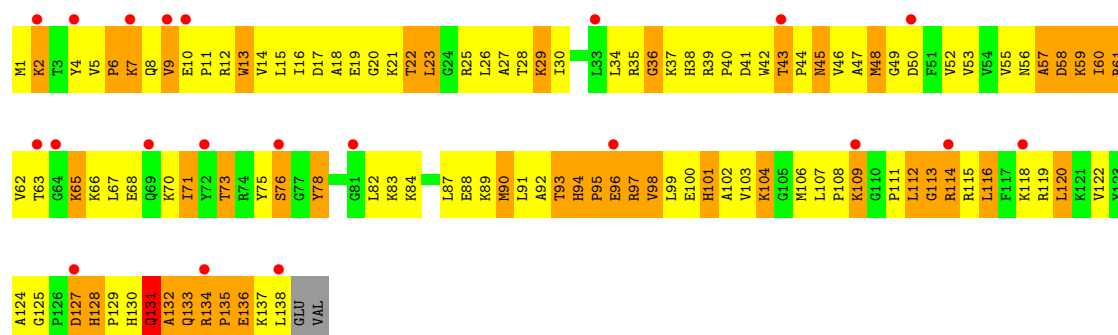
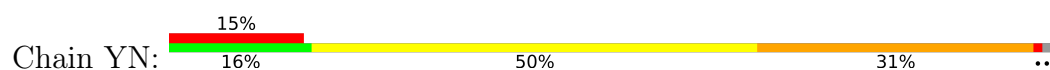


• Molecule 33: 50S ribosomal protein L13

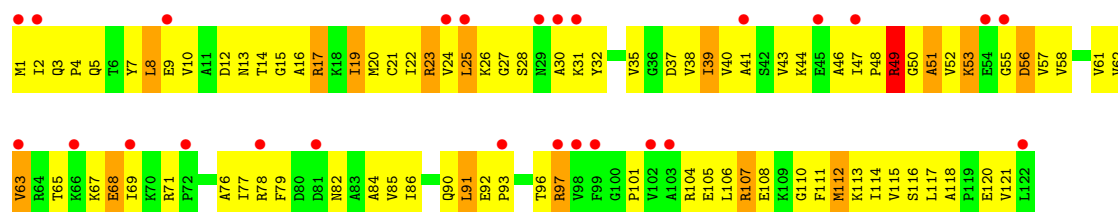




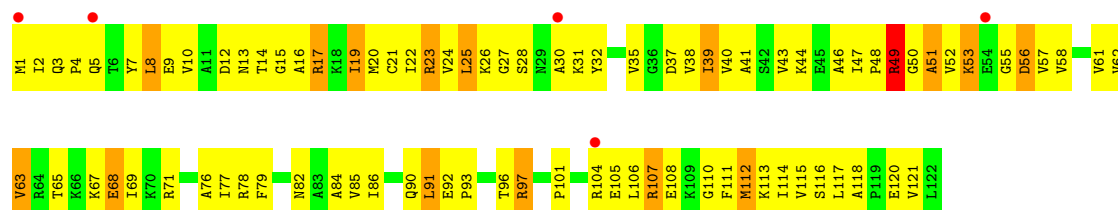
• Molecule 33: 50S ribosomal protein L13



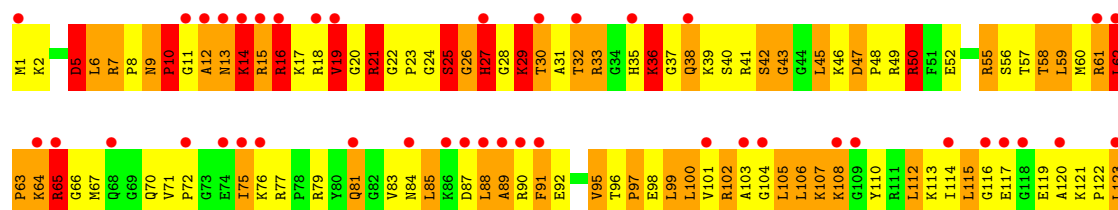
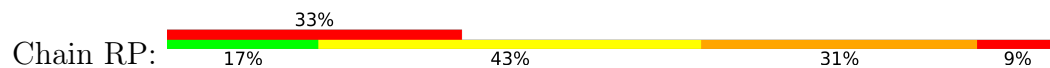
• Molecule 34: 50S ribosomal protein L14

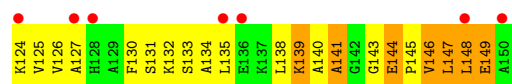


• Molecule 34: 50S ribosomal protein L14

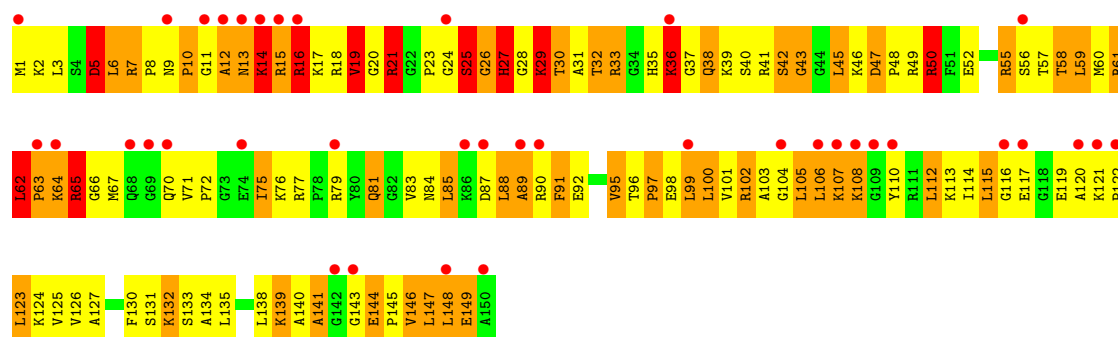
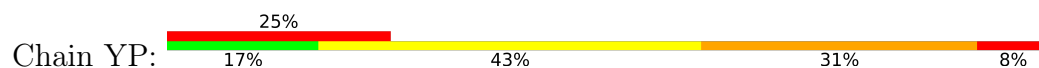


• Molecule 35: 50S ribosomal protein L15

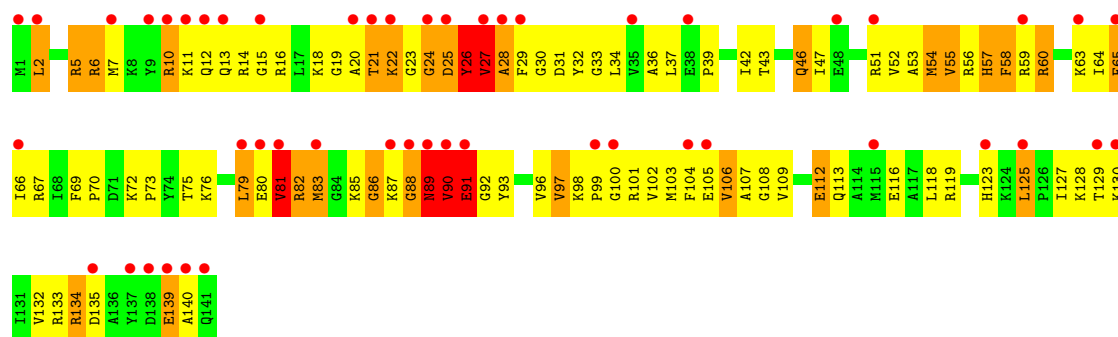




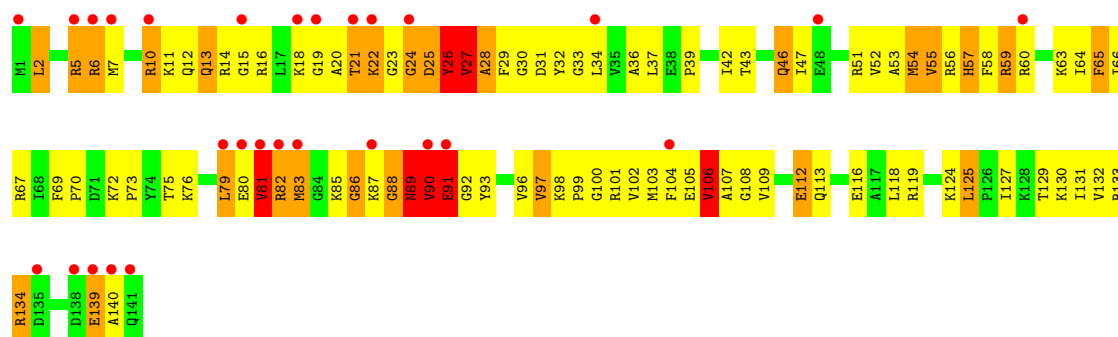
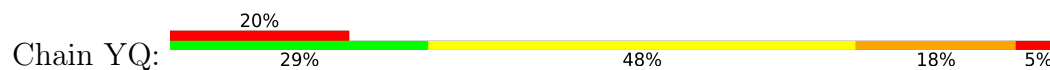
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

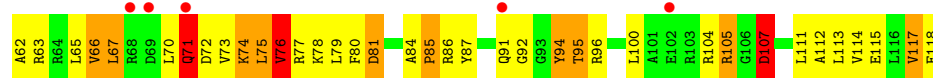
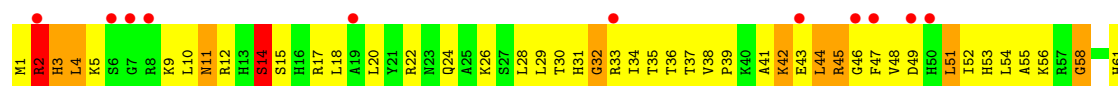


• Molecule 36: 50S ribosomal protein L16

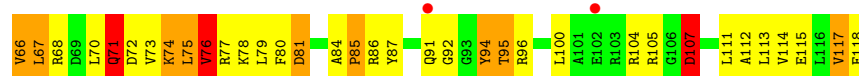
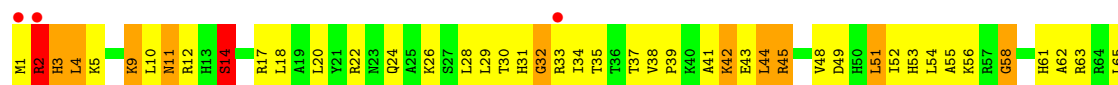


• Molecule 37: 50S ribosomal protein L17

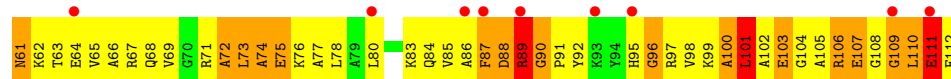
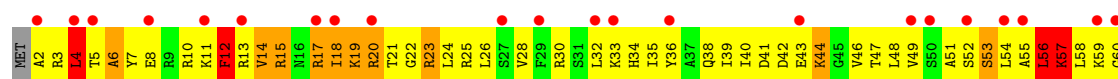
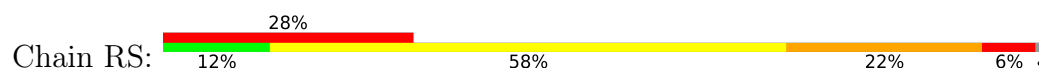




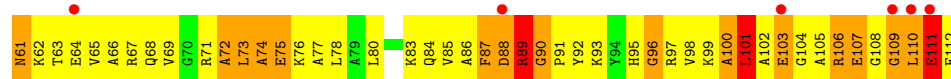
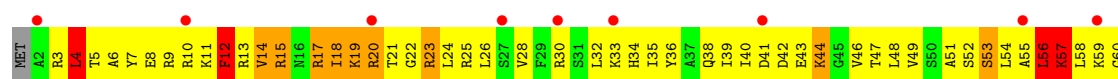
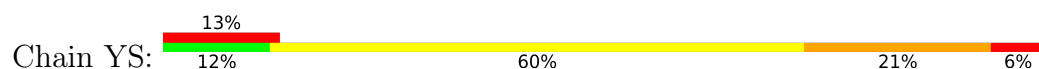
• Molecule 37: 50S ribosomal protein L17



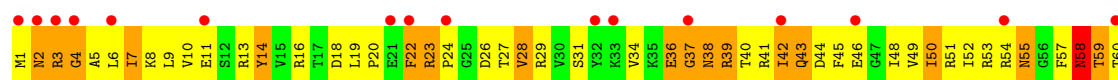
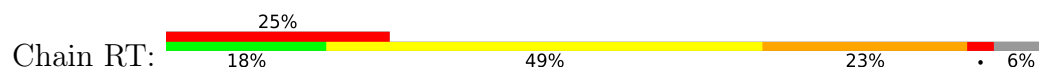
• Molecule 38: 50S ribosomal protein L18

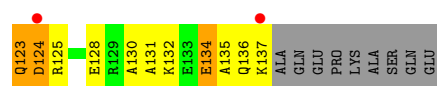


• Molecule 38: 50S ribosomal protein L18

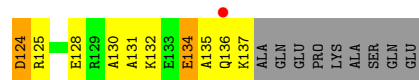
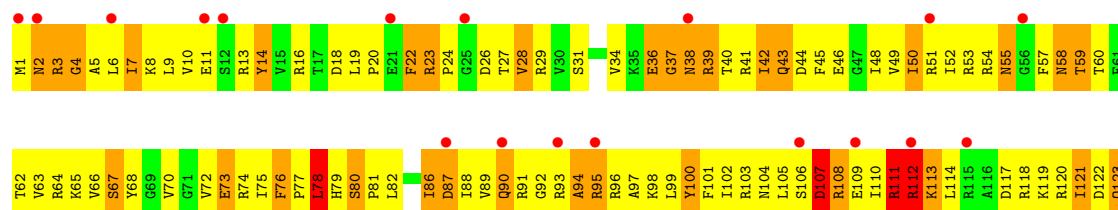
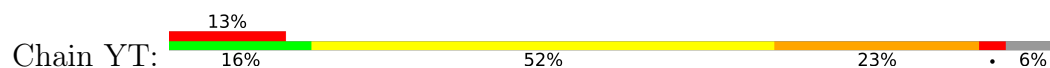


• Molecule 39: 50S ribosomal protein L19

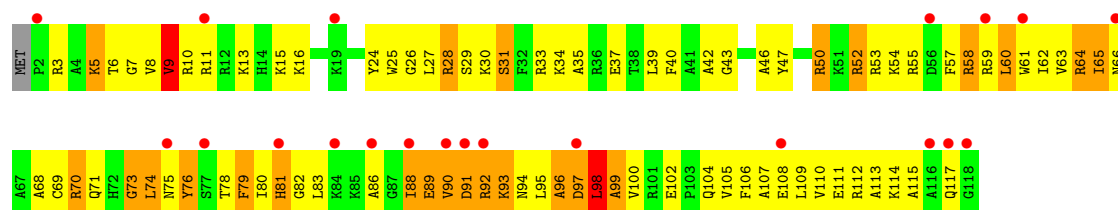




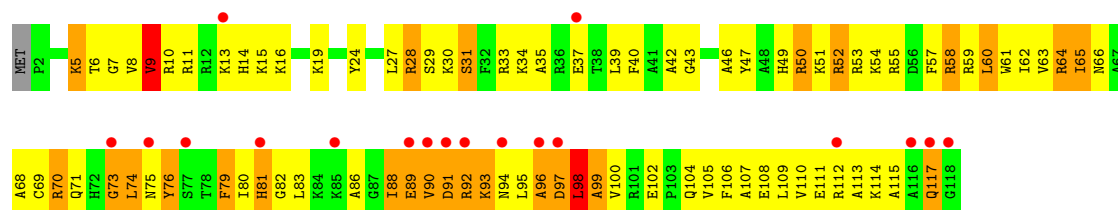
• Molecule 39: 50S ribosomal protein L19



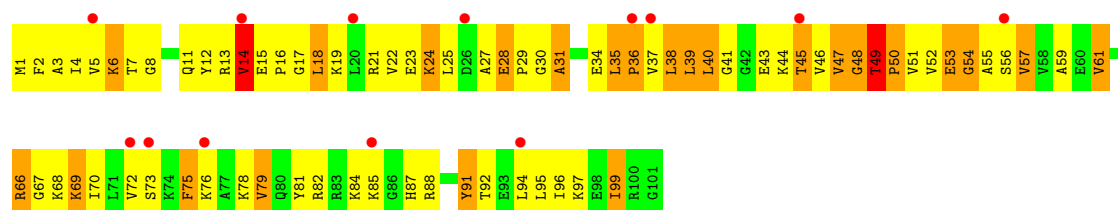
• Molecule 40: 50S ribosomal protein L20



• Molecule 40: 50S ribosomal protein L20

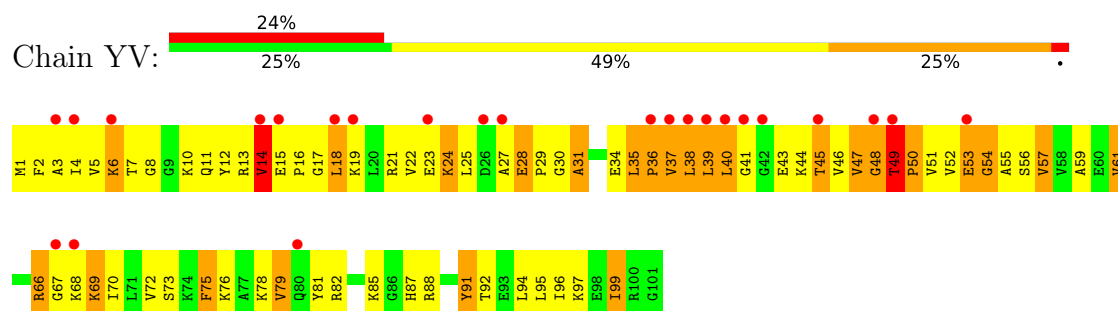


• Molecule 41: 50S ribosomal protein L21

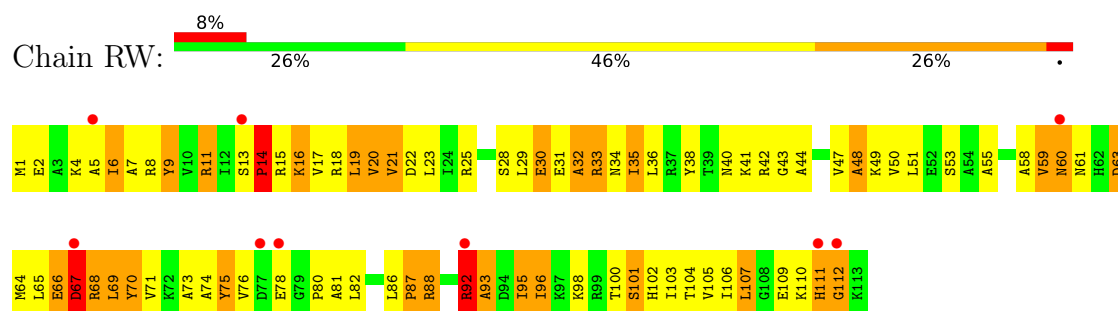




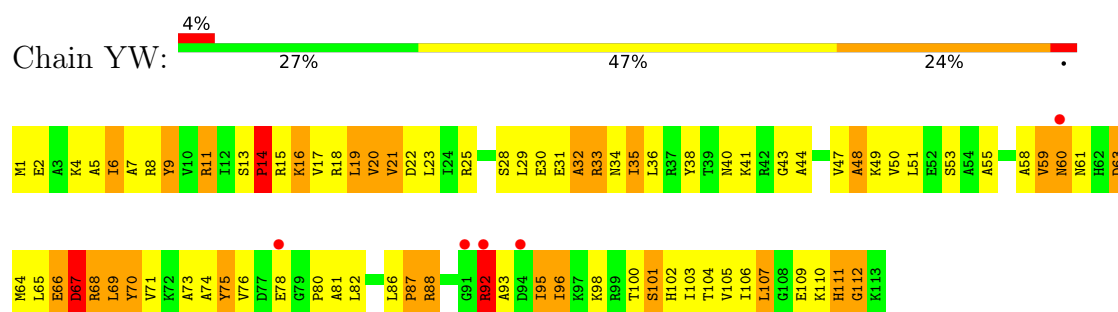
- Molecule 41: 50S ribosomal protein L21



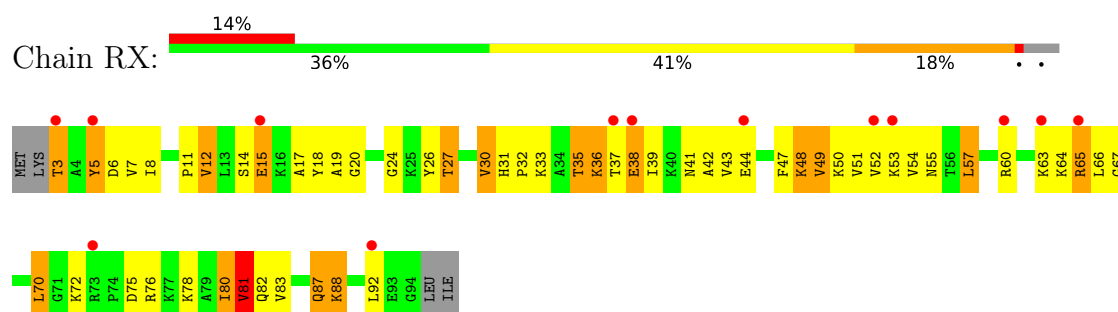
- Molecule 42: 50S ribosomal protein L22



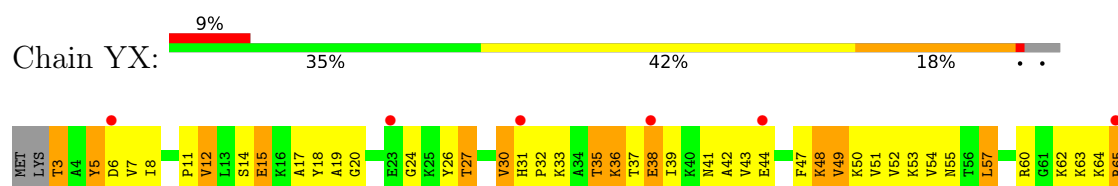
- Molecule 42: 50S ribosomal protein L22

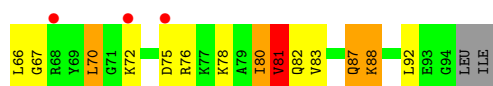


- Molecule 43: 50S ribosomal protein L23

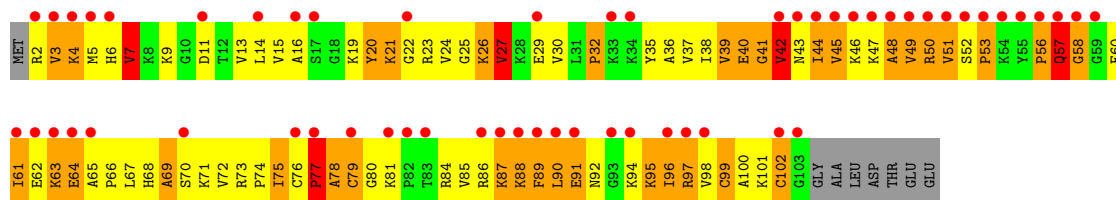
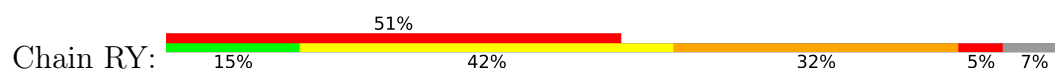


- Molecule 43: 50S ribosomal protein L23

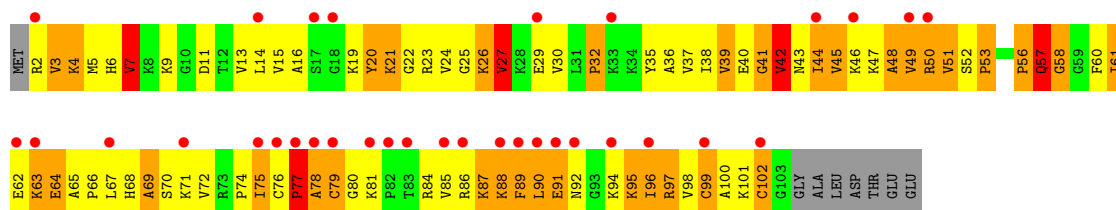
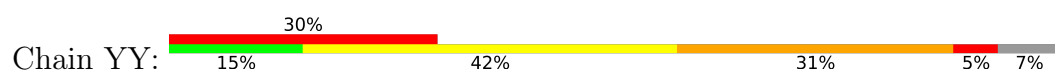




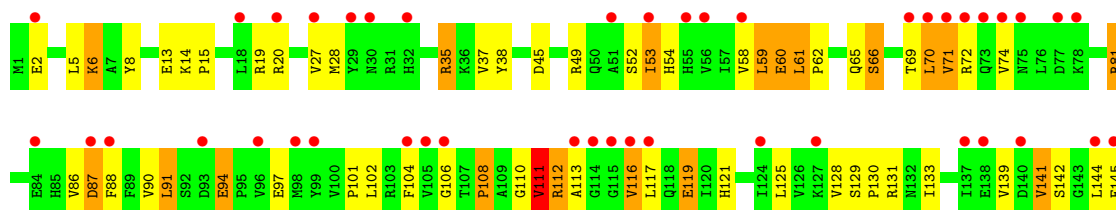
- Molecule 44: 50S ribosomal protein L24



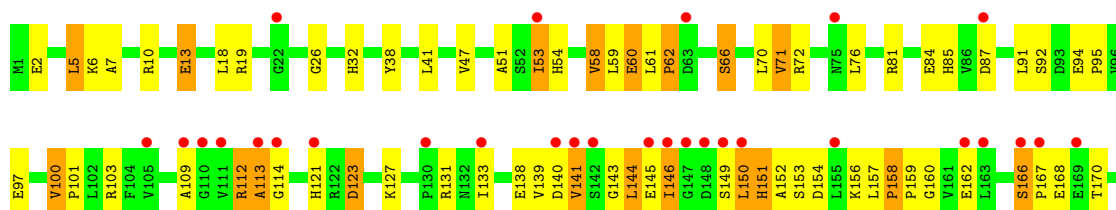
- Molecule 44: 50S ribosomal protein L24

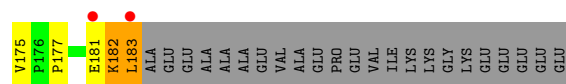


- Molecule 45: 50S ribosomal protein L25

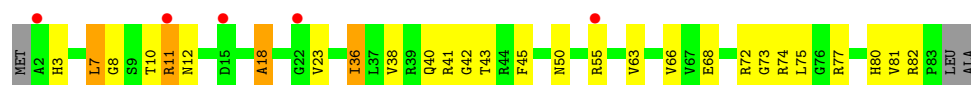


- Molecule 45: 50S ribosomal protein L25

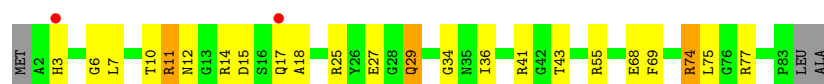




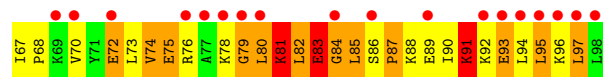
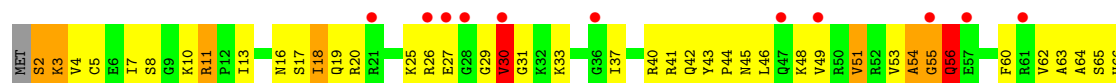
- Molecule 46: 50S ribosomal protein L27



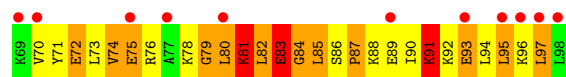
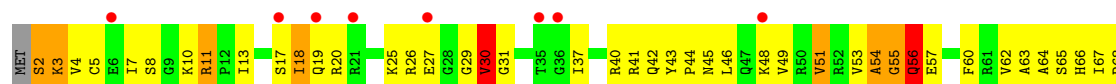
- Molecule 46: 50S ribosomal protein L27



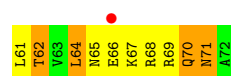
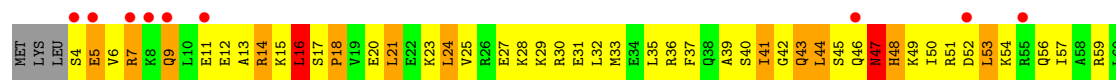
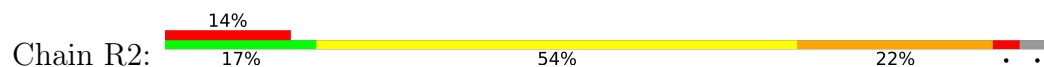
- Molecule 47: 50S ribosomal protein L28



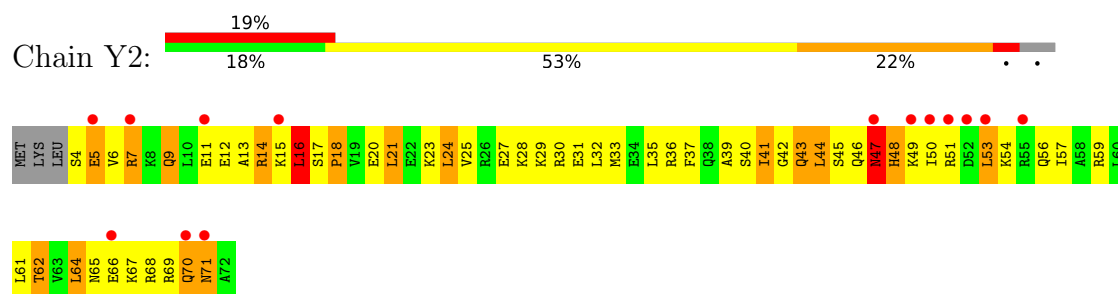
- Molecule 47: 50S ribosomal protein L28



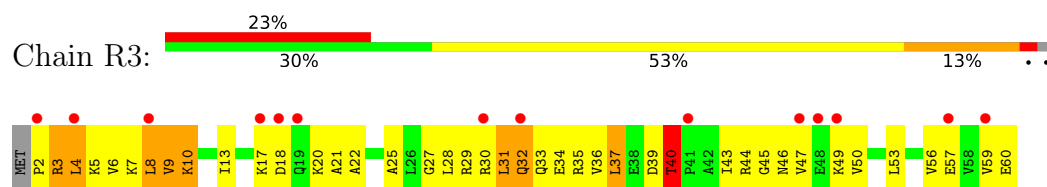
- Molecule 48: 50S ribosomal protein L29



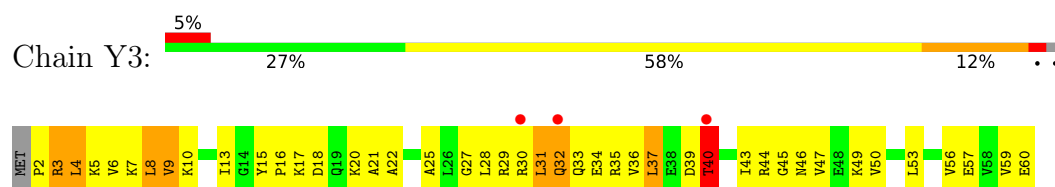
- Molecule 48: 50S ribosomal protein L29



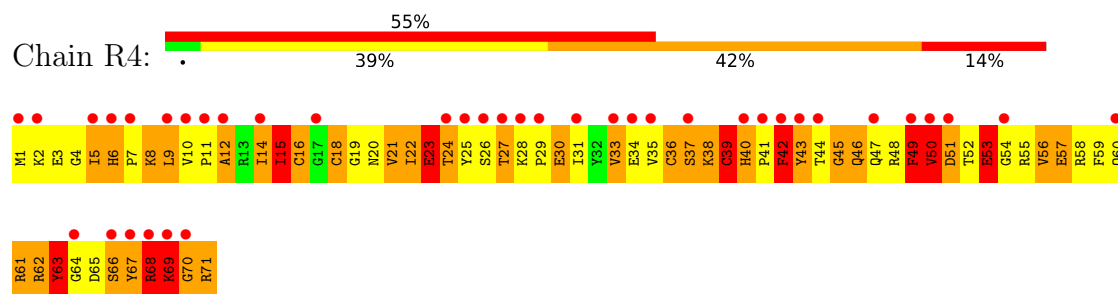
- Molecule 49: 50S ribosomal protein L30



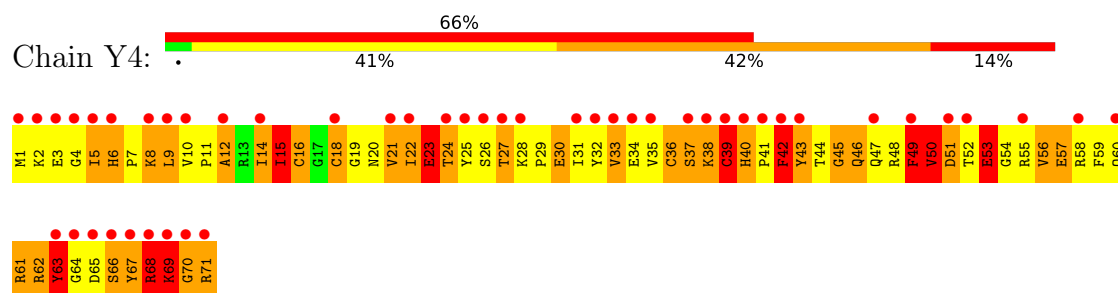
- Molecule 49: 50S ribosomal protein L30



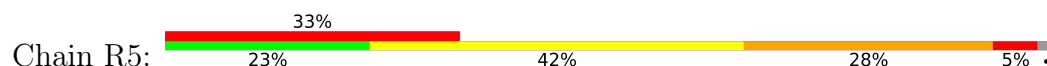
- Molecule 50: 50S ribosomal protein L31

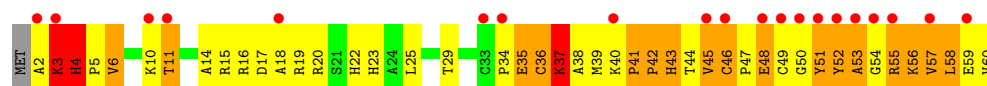


- Molecule 50: 50S ribosomal protein L31

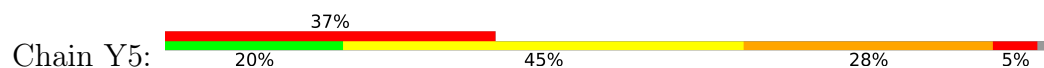


- Molecule 51: 50S ribosomal protein L32

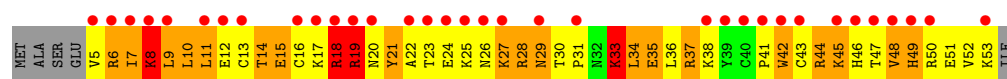




- Molecule 51: 50S ribosomal protein L32



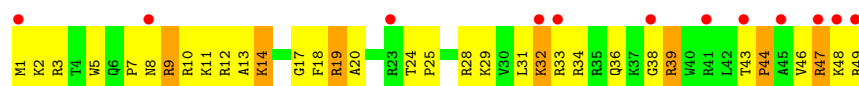
- Molecule 52: 50S ribosomal protein L33



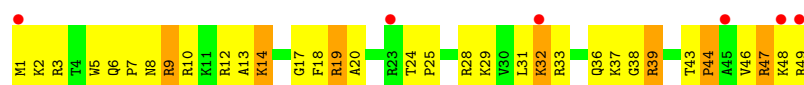
- Molecule 52: 50S ribosomal protein L33



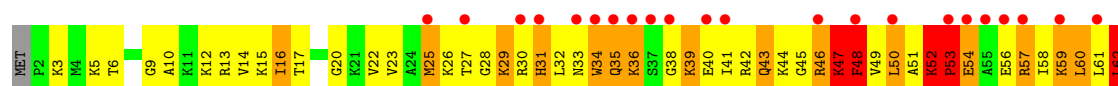
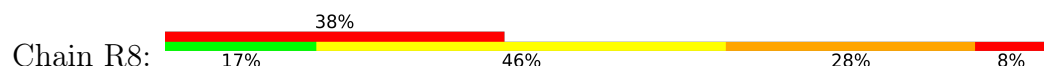
- Molecule 53: 50S ribosomal protein L34



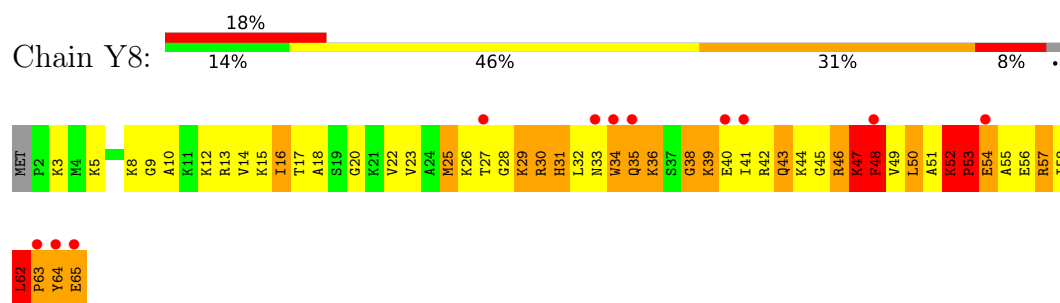
- Molecule 53: 50S ribosomal protein L34



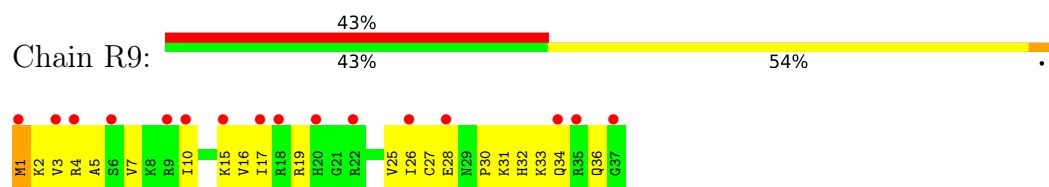
- Molecule 54: 50S ribosomal protein L35



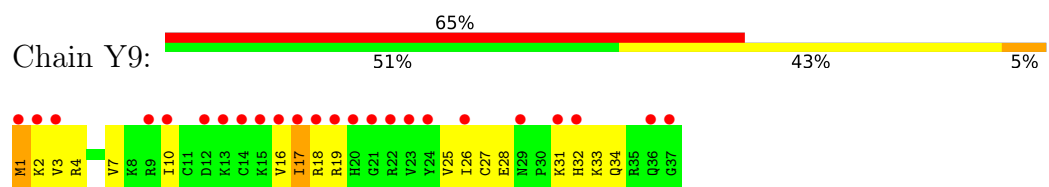
- Molecule 54: 50S ribosomal protein L35



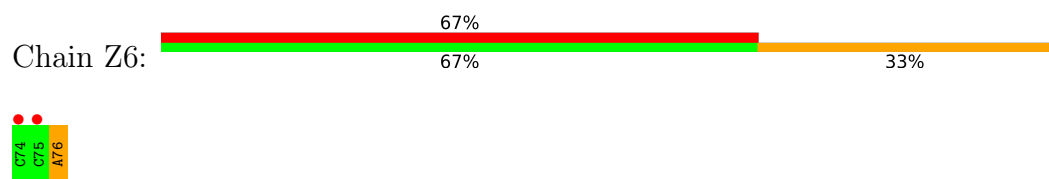
- Molecule 55: 50S ribosomal protein L36



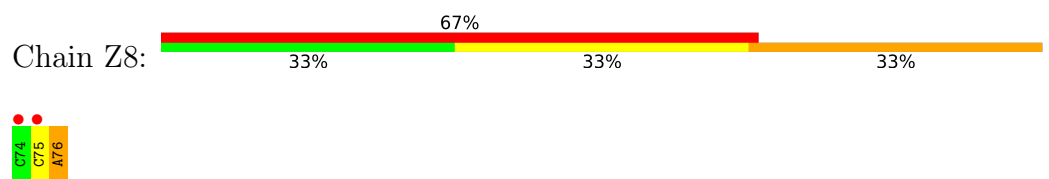
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 208.25Å 448.40Å 624.58Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 34.97 – 3.48<br>34.97 – 3.48                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (34.97-3.48)<br>99.5 (34.97-3.48)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.32                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.61 (at 3.32Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.230 , 0.270<br>0.231 , 0.269                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 39762 reflections (4.62%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.303                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 73.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 292002                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                        | 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: PAR, PPU, MG, ZN, 1MG

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    | 0.18         | 0/36098      | 0.38        | 0/56341        |
| 1   | XA    | 0.20         | 0/36101      | 0.40        | 0/56346        |
| 2   | QB    | 0.42         | 0/1959       | 1.05        | 11/2642 (0.4%) |
| 2   | XB    | 0.42         | 0/1959       | 1.07        | 11/2642 (0.4%) |
| 3   | QC    | 0.44         | 0/1629       | 0.92        | 1/2195 (0.0%)  |
| 3   | XC    | 0.44         | 0/1629       | 0.93        | 1/2195 (0.0%)  |
| 4   | QD    | 0.49         | 0/1733       | 1.06        | 12/2318 (0.5%) |
| 4   | XD    | 0.55         | 0/1733       | 1.06        | 14/2318 (0.6%) |
| 5   | QE    | 0.46         | 0/1171       | 1.02        | 9/1576 (0.6%)  |
| 5   | XE    | 0.46         | 0/1171       | 1.02        | 9/1576 (0.6%)  |
| 6   | QF    | 0.50         | 0/856        | 0.97        | 3/1154 (0.3%)  |
| 6   | XF    | 0.50         | 0/856        | 0.97        | 3/1154 (0.3%)  |
| 7   | QG    | 0.43         | 0/1276       | 0.90        | 1/1709 (0.1%)  |
| 7   | XG    | 0.42         | 0/1276       | 0.90        | 1/1709 (0.1%)  |
| 8   | QH    | 0.49         | 0/1136       | 1.05        | 5/1527 (0.3%)  |
| 8   | XH    | 0.50         | 0/1136       | 1.06        | 7/1527 (0.5%)  |
| 9   | QI    | 0.40         | 0/1029       | 1.02        | 8/1379 (0.6%)  |
| 9   | XI    | 0.40         | 0/1029       | 1.03        | 9/1379 (0.7%)  |
| 10  | QJ    | 0.47         | 0/814        | 0.91        | 1/1095 (0.1%)  |
| 10  | XJ    | 0.47         | 0/814        | 0.91        | 1/1095 (0.1%)  |
| 11  | QK    | 0.47         | 0/900        | 1.05        | 6/1213 (0.5%)  |
| 11  | XK    | 0.48         | 0/900        | 1.04        | 6/1213 (0.5%)  |
| 12  | QL    | 0.55         | 0/991        | 1.74        | 11/1327 (0.8%) |
| 12  | XL    | 0.55         | 0/991        | 1.74        | 11/1327 (0.8%) |
| 13  | QM    | 0.44         | 0/974        | 1.05        | 9/1303 (0.7%)  |
| 13  | XM    | 0.43         | 0/974        | 1.05        | 9/1303 (0.7%)  |
| 14  | QN    | 0.47         | 0/501        | 1.08        | 6/664 (0.9%)   |
| 14  | XN    | 0.65         | 1/501 (0.2%) | 1.07        | 4/664 (0.6%)   |
| 15  | QO    | 0.48         | 0/745        | 0.99        | 3/992 (0.3%)   |
| 15  | XO    | 0.48         | 0/745        | 0.99        | 3/992 (0.3%)   |
| 16  | QP    | 0.46         | 0/721        | 1.03        | 4/970 (0.4%)   |
| 16  | XP    | 0.46         | 0/721        | 1.04        | 4/970 (0.4%)   |



| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 17  | QQ    | 0.42         | 0/847         | 1.07        | 6/1131 (0.5%)   |
| 17  | XQ    | 0.44         | 0/847         | 1.06        | 6/1131 (0.5%)   |
| 18  | QR    | 0.47         | 0/579         | 1.04        | 3/768 (0.4%)    |
| 18  | XR    | 0.47         | 0/579         | 1.04        | 3/768 (0.4%)    |
| 19  | QS    | 0.46         | 0/689         | 1.21        | 7/926 (0.8%)    |
| 19  | XS    | 0.46         | 0/689         | 1.21        | 7/926 (0.8%)    |
| 20  | QT    | 0.42         | 0/765         | 1.09        | 6/1007 (0.6%)   |
| 20  | XT    | 0.42         | 0/765         | 1.09        | 4/1007 (0.4%)   |
| 21  | QU    | 0.42         | 0/221         | 1.01        | 1/288 (0.3%)    |
| 21  | XU    | 0.42         | 0/221         | 1.01        | 1/288 (0.3%)    |
| 22  | QV    | 0.34         | 1/1836 (0.1%) | 0.43        | 0/2859          |
| 22  | XV    | 0.34         | 1/1836 (0.1%) | 0.43        | 0/2859          |
| 23  | QY    | 0.34         | 0/333         | 0.74        | 1/517 (0.2%)    |
| 23  | XY    | 0.35         | 0/333         | 0.74        | 1/517 (0.2%)    |
| 24  | QX    | 0.84         | 2/193 (1.0%)  | 1.21        | 3/299 (1.0%)    |
| 24  | XX    | 0.84         | 2/193 (1.0%)  | 1.21        | 3/299 (1.0%)    |
| 25  | RA    | 0.21         | 0/69521       | 0.40        | 3/108529 (0.0%) |
| 25  | YA    | 0.24         | 0/69543       | 0.43        | 3/108563 (0.0%) |
| 26  | RB    | 0.18         | 0/2878        | 0.35        | 0/4490          |
| 26  | YB    | 0.21         | 0/2878        | 0.40        | 0/4490          |
| 27  | RD    | 0.79         | 2/2165 (0.1%) | 1.30        | 34/2919 (1.2%)  |
| 27  | YD    | 0.72         | 1/2165 (0.0%) | 1.30        | 32/2919 (1.1%)  |
| 28  | RE    | 0.62         | 0/1601        | 1.35        | 29/2160 (1.3%)  |
| 28  | YE    | 0.62         | 0/1601        | 1.35        | 29/2160 (1.3%)  |
| 29  | RF    | 0.62         | 0/1620        | 1.19        | 18/2194 (0.8%)  |
| 29  | YF    | 0.62         | 0/1620        | 1.20        | 16/2194 (0.7%)  |
| 30  | RG    | 0.47         | 0/1499        | 0.99        | 9/2016 (0.4%)   |
| 30  | YG    | 0.47         | 0/1499        | 0.99        | 9/2016 (0.4%)   |
| 31  | RH    | 0.57         | 0/1332        | 1.22        | 14/1802 (0.8%)  |
| 31  | YH    | 0.58         | 0/1332        | 1.22        | 15/1802 (0.8%)  |
| 32  | RI    | 0.48         | 0/1151        | 0.90        | 2/1558 (0.1%)   |
| 32  | YI    | 0.44         | 0/1151        | 0.94        | 3/1558 (0.2%)   |
| 33  | RN    | 0.55         | 0/1131        | 1.18        | 10/1525 (0.7%)  |
| 33  | YN    | 0.55         | 0/1131        | 1.18        | 10/1525 (0.7%)  |
| 34  | RO    | 0.65         | 0/943         | 1.04        | 5/1269 (0.4%)   |
| 34  | YO    | 0.65         | 0/943         | 1.04        | 5/1269 (0.4%)   |
| 35  | RP    | 0.63         | 0/1162        | 1.37        | 17/1544 (1.1%)  |
| 35  | YP    | 0.63         | 1/1162 (0.1%) | 1.37        | 17/1544 (1.1%)  |
| 36  | RQ    | 0.71         | 0/1143        | 1.36        | 19/1527 (1.2%)  |
| 36  | YQ    | 0.71         | 0/1143        | 1.35        | 19/1527 (1.2%)  |
| 37  | RR    | 0.55         | 0/982         | 1.17        | 10/1312 (0.8%)  |
| 37  | YR    | 0.55         | 0/982         | 1.17        | 10/1312 (0.8%)  |
| 38  | RS    | 0.53         | 0/892         | 1.18        | 8/1187 (0.7%)   |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | YS    | 0.52         | 0/892            | 1.18        | 8/1187 (0.7%)     |
| 39  | RT    | 0.56         | 0/1155           | 1.18        | 16/1542 (1.0%)    |
| 39  | YT    | 0.56         | 0/1155           | 1.18        | 17/1542 (1.1%)    |
| 40  | RU    | 0.59         | 0/982            | 1.21        | 10/1306 (0.8%)    |
| 40  | YU    | 0.60         | 0/982            | 1.21        | 10/1306 (0.8%)    |
| 41  | RV    | 0.56         | 0/790            | 1.10        | 6/1057 (0.6%)     |
| 41  | YV    | 0.56         | 0/790            | 1.10        | 6/1057 (0.6%)     |
| 42  | RW    | 0.58         | 0/911            | 1.18        | 13/1220 (1.1%)    |
| 42  | YW    | 0.58         | 0/911            | 1.18        | 12/1220 (1.0%)    |
| 43  | RX    | 0.62         | 0/739            | 1.13        | 5/993 (0.5%)      |
| 43  | YX    | 0.62         | 0/739            | 1.14        | 5/993 (0.5%)      |
| 44  | RY    | 0.65         | 0/798            | 1.17        | 4/1064 (0.4%)     |
| 44  | YY    | 0.64         | 0/798            | 1.16        | 3/1064 (0.3%)     |
| 45  | RZ    | 0.40         | 0/1493           | 0.92        | 4/2026 (0.2%)     |
| 45  | YZ    | 0.44         | 0/1493           | 0.94        | 5/2026 (0.2%)     |
| 46  | R0    | 0.37         | 0/657            | 0.80        | 0/874             |
| 46  | Y0    | 0.53         | 1/657 (0.2%)     | 0.82        | 0/874             |
| 47  | R1    | 0.58         | 0/770            | 1.20        | 9/1022 (0.9%)     |
| 47  | Y1    | 0.58         | 0/770            | 1.20        | 9/1022 (0.9%)     |
| 48  | R2    | 0.61         | 0/583            | 1.32        | 9/771 (1.2%)      |
| 48  | Y2    | 0.61         | 0/583            | 1.32        | 8/771 (1.0%)      |
| 49  | R3    | 0.62         | 1/474 (0.2%)     | 1.04        | 0/635             |
| 49  | Y3    | 0.54         | 0/474            | 1.04        | 0/635             |
| 50  | R4    | 0.47         | 0/594            | 1.24        | 10/795 (1.3%)     |
| 50  | Y4    | 0.47         | 0/594            | 1.24        | 10/795 (1.3%)     |
| 51  | R5    | 0.65         | 0/473            | 1.21        | 6/639 (0.9%)      |
| 51  | Y5    | 0.65         | 0/473            | 1.22        | 7/639 (1.1%)      |
| 52  | R6    | 0.54         | 0/431            | 1.06        | 3/575 (0.5%)      |
| 52  | Y6    | 0.53         | 0/431            | 1.06        | 3/575 (0.5%)      |
| 53  | R7    | 0.73         | 0/438            | 1.19        | 2/575 (0.3%)      |
| 53  | Y7    | 0.74         | 0/438            | 1.19        | 2/575 (0.3%)      |
| 54  | R8    | 0.79         | 0/525            | 1.41        | 9/691 (1.3%)      |
| 54  | Y8    | 0.80         | 0/525            | 1.41        | 9/691 (1.3%)      |
| 55  | R9    | 0.43         | 0/310            | 0.92        | 1/407 (0.2%)      |
| 55  | Y9    | 0.45         | 0/310            | 0.92        | 1/407 (0.2%)      |
| 56  | Z6    | 0.46         | 0/40             | 0.62        | 0/60              |
| 56  | Z8    | 0.46         | 0/40             | 0.62        | 0/60              |
| All | All   | 0.35         | 13/316383 (0.0%) | 0.69        | 803/473007 (0.2%) |

All (13) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | RD    | 236 | GLY  | C-N     | 14.33 | 1.53        | 1.33     |
| 24  | XX    | 7   | G    | C1'-N9  | -6.68 | 1.38        | 1.48     |
| 24  | QX    | 7   | G    | C1'-N9  | -6.61 | 1.38        | 1.48     |
| 24  | XX    | 6   | G    | C1'-N9  | -6.38 | 1.38        | 1.48     |
| 22  | QV    | 1   | C    | OP3-P   | 6.36  | 1.61        | 1.48     |
| 24  | QX    | 6   | G    | C1'-N9  | -6.35 | 1.38        | 1.48     |
| 22  | XV    | 1   | C    | OP3-P   | 6.34  | 1.61        | 1.48     |
| 46  | Y0    | 3   | HIS  | CE1-NE2 | 5.69  | 1.38        | 1.32     |
| 49  | R3    | 10  | LYS  | C-O     | -5.53 | 1.17        | 1.23     |
| 14  | XN    | 25  | VAL  | C-N     | 5.27  | 1.43        | 1.33     |
| 27  | RD    | 241 | PRO  | N-CD    | 5.24  | 1.55        | 1.47     |
| 35  | YP    | 19  | VAL  | CA-C    | 5.09  | 1.59        | 1.52     |
| 27  | YD    | 241 | PRO  | N-CD    | 5.01  | 1.54        | 1.47     |

All (803) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 12  | XL    | 47  | LYS  | CA-C-N    | 31.30  | 158.96      | 119.84   |
| 12  | XL    | 47  | LYS  | C-N-CA    | 31.30  | 158.96      | 119.84   |
| 12  | QL    | 47  | LYS  | CA-C-N    | 31.28  | 158.94      | 119.84   |
| 12  | QL    | 47  | LYS  | C-N-CA    | 31.28  | 158.94      | 119.84   |
| 35  | RP    | 59  | LEU  | N-CA-C    | -14.62 | 91.39       | 111.56   |
| 35  | YP    | 59  | LEU  | N-CA-C    | -14.61 | 91.40       | 111.56   |
| 50  | Y4    | 39  | CYS  | N-CA-C    | -13.57 | 95.99       | 112.54   |
| 50  | R4    | 39  | CYS  | N-CA-C    | -13.52 | 96.04       | 112.54   |
| 23  | QY    | 40  | G    | P-O3'-C3' | -13.32 | 100.23      | 120.20   |
| 23  | XY    | 40  | G    | P-O3'-C3' | -13.28 | 100.28      | 120.20   |
| 24  | XX    | 7   | G    | O3'-P-O5' | 13.00  | 123.50      | 104.00   |
| 24  | QX    | 7   | G    | O3'-P-O5' | 12.94  | 123.41      | 104.00   |
| 12  | QL    | 47  | LYS  | C-N-CD    | -12.07 | 75.52       | 125.00   |
| 12  | XL    | 47  | LYS  | C-N-CD    | -12.05 | 75.61       | 125.00   |
| 28  | RE    | 58  | ARG  | N-CA-C    | -11.82 | 95.21       | 113.89   |
| 28  | YE    | 58  | ARG  | N-CA-C    | -11.82 | 95.21       | 113.89   |
| 48  | R2    | 5   | GLU  | N-CA-C    | -11.63 | 99.58       | 113.88   |
| 48  | Y2    | 5   | GLU  | N-CA-C    | -11.59 | 99.62       | 113.88   |
| 33  | RN    | 114 | ARG  | N-CA-C    | -11.46 | 95.98       | 110.19   |
| 40  | YU    | 96  | ALA  | N-CA-C    | -11.46 | 98.73       | 113.17   |
| 40  | RU    | 96  | ALA  | N-CA-C    | -11.44 | 98.76       | 113.17   |
| 33  | YN    | 114 | ARG  | N-CA-C    | -11.43 | 96.02       | 110.19   |
| 52  | R6    | 29  | ASN  | N-CA-C    | -10.64 | 99.04       | 113.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 52  | Y6    | 29  | ASN  | N-CA-C    | -10.63 | 99.06       | 113.30   |
| 36  | RQ    | 89  | ASN  | N-CA-C    | -10.38 | 100.42      | 112.87   |
| 12  | QL    | 119 | LYS  | N-CA-C    | -10.34 | 95.22       | 110.52   |
| 12  | XL    | 119 | LYS  | N-CA-C    | -10.32 | 95.24       | 110.52   |
| 36  | YQ    | 89  | ASN  | N-CA-C    | -10.25 | 100.57      | 112.87   |
| 28  | YE    | 21  | VAL  | C-N-CD    | -10.15 | 98.26       | 120.60   |
| 28  | RE    | 21  | VAL  | C-N-CD    | -10.06 | 98.47       | 120.60   |
| 36  | YQ    | 81  | VAL  | CB-CA-C   | -10.00 | 94.88       | 111.29   |
| 2   | QB    | 25  | ASN  | CA-C-N    | 9.98   | 132.31      | 119.84   |
| 2   | QB    | 25  | ASN  | C-N-CA    | 9.98   | 132.31      | 119.84   |
| 36  | YQ    | 81  | VAL  | N-CA-C    | 9.96   | 130.05      | 109.34   |
| 2   | XB    | 25  | ASN  | CA-C-N    | 9.94   | 132.26      | 119.84   |
| 2   | XB    | 25  | ASN  | C-N-CA    | 9.94   | 132.26      | 119.84   |
| 36  | RQ    | 81  | VAL  | CB-CA-C   | -9.92  | 95.02       | 111.29   |
| 36  | RQ    | 81  | VAL  | N-CA-C    | 9.92   | 129.97      | 109.34   |
| 35  | RP    | 13  | ASN  | N-CA-C    | -9.68  | 101.49      | 113.20   |
| 35  | YP    | 13  | ASN  | N-CA-C    | -9.61  | 101.57      | 113.20   |
| 24  | QX    | 7   | G    | OP1-P-O3' | -9.48  | 79.55       | 108.00   |
| 24  | XX    | 7   | G    | OP1-P-O3' | -9.46  | 79.61       | 108.00   |
| 29  | YF    | 197 | ASP  | N-CA-C    | -9.26  | 98.70       | 110.19   |
| 29  | RF    | 197 | ASP  | N-CA-C    | -9.25  | 98.72       | 110.19   |
| 12  | QL    | 26  | ALA  | N-CA-C    | -9.24  | 102.58      | 113.21   |
| 11  | QK    | 40  | ILE  | N-CA-C    | -9.18  | 103.66      | 111.56   |
| 12  | XL    | 26  | ALA  | N-CA-C    | -9.14  | 102.70      | 113.21   |
| 50  | Y4    | 45  | GLY  | N-CA-C    | -9.10  | 102.77      | 115.32   |
| 50  | R4    | 45  | GLY  | N-CA-C    | -9.08  | 102.79      | 115.32   |
| 38  | YS    | 110 | LEU  | CB-CA-C   | -8.96  | 105.05      | 117.23   |
| 11  | XK    | 40  | ILE  | N-CA-C    | -8.94  | 103.87      | 111.56   |
| 47  | R1    | 3   | LYS  | N-CA-C    | -8.89  | 99.77       | 110.44   |
| 47  | Y1    | 3   | LYS  | N-CA-C    | -8.89  | 99.77       | 110.44   |
| 53  | Y7    | 47  | ARG  | N-CA-C    | 8.88   | 119.65      | 108.19   |
| 38  | RS    | 110 | LEU  | CB-CA-C   | -8.87  | 105.17      | 117.23   |
| 53  | R7    | 47  | ARG  | N-CA-C    | 8.85   | 119.61      | 108.19   |
| 40  | RU    | 97  | ASP  | N-CA-C    | -8.78  | 103.66      | 112.97   |
| 27  | RD    | 91  | ARG  | N-CA-C    | -8.77  | 98.71       | 110.55   |
| 40  | YU    | 97  | ASP  | N-CA-C    | -8.73  | 103.71      | 112.97   |
| 27  | YD    | 91  | ARG  | N-CA-C    | -8.72  | 98.78       | 110.55   |
| 40  | RU    | 98  | LEU  | N-CA-C    | -8.70  | 102.47      | 113.43   |
| 40  | YU    | 98  | LEU  | N-CA-C    | -8.68  | 102.49      | 113.43   |
| 36  | RQ    | 125 | LEU  | CA-C-N    | 8.67   | 130.67      | 119.84   |
| 36  | RQ    | 125 | LEU  | C-N-CA    | 8.67   | 130.67      | 119.84   |
| 54  | Y8    | 36  | LYS  | N-CA-C    | -8.67  | 96.70       | 110.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 36  | YQ    | 125 | LEU  | CA-C-N | 8.64  | 130.64      | 119.84   |
| 36  | YQ    | 125 | LEU  | C-N-CA | 8.64  | 130.64      | 119.84   |
| 54  | R8    | 36  | LYS  | N-CA-C | -8.62 | 96.77       | 110.14   |
| 28  | RE    | 23  | VAL  | N-CA-C | 8.52  | 121.05      | 108.96   |
| 8   | XH    | 79  | VAL  | N-CA-C | -8.50 | 102.13      | 110.72   |
| 37  | RR    | 9   | LYS  | N-CA-C | -8.47 | 94.71       | 108.52   |
| 28  | YE    | 23  | VAL  | N-CA-C | 8.47  | 120.98      | 108.96   |
| 8   | QH    | 79  | VAL  | N-CA-C | -8.41 | 102.22      | 110.72   |
| 39  | YT    | 59  | THR  | N-CA-C | -8.41 | 97.39       | 110.42   |
| 39  | RT    | 59  | THR  | N-CA-C | -8.40 | 97.40       | 110.42   |
| 37  | YR    | 9   | LYS  | N-CA-C | -8.39 | 94.84       | 108.52   |
| 16  | QP    | 3   | LYS  | N-CA-C | 8.34  | 120.61      | 108.86   |
| 39  | RT    | 7   | ILE  | N-CA-C | -8.33 | 101.56      | 110.23   |
| 47  | R1    | 79  | GLY  | N-CA-C | -8.30 | 93.50       | 113.18   |
| 16  | XP    | 3   | LYS  | N-CA-C | 8.30  | 120.57      | 108.86   |
| 29  | RF    | 75  | HIS  | N-CA-C | 8.30  | 122.38      | 109.52   |
| 27  | RD    | 193 | VAL  | N-CA-C | 8.28  | 120.26      | 109.58   |
| 47  | Y1    | 79  | GLY  | N-CA-C | -8.26 | 93.60       | 113.18   |
| 39  | YT    | 13  | ARG  | N-CA-C | -8.25 | 102.66      | 114.12   |
| 29  | YF    | 75  | HIS  | N-CA-C | 8.23  | 122.28      | 109.52   |
| 39  | YT    | 7   | ILE  | N-CA-C | -8.22 | 101.68      | 110.23   |
| 34  | RO    | 107 | ARG  | N-CA-C | -8.22 | 102.27      | 111.07   |
| 34  | YO    | 107 | ARG  | N-CA-C | -8.19 | 102.31      | 111.07   |
| 39  | RT    | 13  | ARG  | N-CA-C | -8.18 | 102.74      | 114.12   |
| 27  | YD    | 193 | VAL  | N-CA-C | 8.17  | 120.12      | 109.58   |
| 29  | YF    | 65  | TRP  | CA-C-N | 8.14  | 130.01      | 119.84   |
| 29  | YF    | 65  | TRP  | C-N-CA | 8.14  | 130.01      | 119.84   |
| 4   | QD    | 72  | GLU  | CA-C-N | -8.12 | 109.93      | 120.65   |
| 4   | QD    | 72  | GLU  | C-N-CA | -8.12 | 109.93      | 120.65   |
| 31  | YH    | 19  | VAL  | N-CA-C | 8.12  | 117.98      | 106.53   |
| 31  | RH    | 19  | VAL  | N-CA-C | 8.09  | 117.93      | 106.53   |
| 29  | RF    | 65  | TRP  | CA-C-N | 8.01  | 129.85      | 119.84   |
| 29  | RF    | 65  | TRP  | C-N-CA | 8.01  | 129.85      | 119.84   |
| 44  | YY    | 20  | TYR  | N-CA-C | -8.01 | 102.00      | 113.21   |
| 50  | R4    | 63  | TYR  | N-CA-C | -7.99 | 102.79      | 112.54   |
| 54  | R8    | 45  | GLY  | N-CA-C | -7.99 | 101.79      | 112.81   |
| 44  | RY    | 20  | TYR  | N-CA-C | -7.96 | 102.06      | 113.21   |
| 54  | Y8    | 45  | GLY  | N-CA-C | -7.93 | 101.87      | 112.81   |
| 34  | YO    | 112 | MET  | N-CA-C | 7.80  | 119.48      | 110.97   |
| 51  | Y5    | 6   | VAL  | CA-C-N | 7.80  | 129.03      | 119.98   |
| 51  | Y5    | 6   | VAL  | C-N-CA | 7.80  | 129.03      | 119.98   |
| 34  | RO    | 112 | MET  | N-CA-C | 7.80  | 119.47      | 110.97   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 51  | R5    | 6   | VAL  | CA-C-N    | 7.79  | 129.02      | 119.98   |
| 51  | R5    | 6   | VAL  | C-N-CA    | 7.79  | 129.02      | 119.98   |
| 36  | RQ    | 5   | ARG  | N-CA-C    | -7.77 | 96.91       | 109.96   |
| 50  | Y4    | 63  | TYR  | N-CA-C    | -7.76 | 102.82      | 111.82   |
| 36  | YQ    | 5   | ARG  | N-CA-C    | -7.76 | 96.93       | 109.96   |
| 20  | QT    | 9   | ASN  | N-CA-C    | 7.75  | 121.95      | 110.48   |
| 37  | RR    | 30  | THR  | N-CA-C    | -7.73 | 105.80      | 114.62   |
| 31  | RH    | 100 | GLY  | N-CA-C    | -7.73 | 99.72       | 111.24   |
| 37  | YR    | 30  | THR  | N-CA-C    | -7.73 | 105.81      | 114.62   |
| 31  | YH    | 100 | GLY  | N-CA-C    | -7.73 | 99.73       | 111.24   |
| 15  | XO    | 78  | TYR  | N-CA-C    | -7.72 | 101.28      | 111.24   |
| 45  | YZ    | 158 | PRO  | CA-C-N    | 7.71  | 129.47      | 119.84   |
| 45  | YZ    | 158 | PRO  | C-N-CA    | 7.71  | 129.47      | 119.84   |
| 15  | QO    | 78  | TYR  | N-CA-C    | -7.70 | 101.31      | 111.24   |
| 4   | XD    | 36  | ARG  | CA-C-N    | 7.70  | 128.66      | 120.12   |
| 4   | XD    | 36  | ARG  | C-N-CA    | 7.70  | 128.66      | 120.12   |
| 24  | XX    | 7   | G    | P-O3'-C3' | -7.69 | 108.67      | 120.20   |
| 24  | QX    | 7   | G    | P-O3'-C3' | -7.67 | 108.69      | 120.20   |
| 4   | QD    | 36  | ARG  | CA-C-N    | 7.65  | 128.61      | 120.12   |
| 4   | QD    | 36  | ARG  | C-N-CA    | 7.65  | 128.61      | 120.12   |
| 11  | XK    | 123 | LYS  | N-CA-C    | -7.64 | 102.55      | 111.03   |
| 11  | QK    | 123 | LYS  | N-CA-C    | -7.63 | 102.56      | 111.03   |
| 54  | Y8    | 38  | GLY  | N-CA-C    | -7.62 | 103.15      | 113.37   |
| 17  | XQ    | 57  | VAL  | N-CA-C    | 7.62  | 118.12      | 108.82   |
| 27  | RD    | 251 | GLY  | N-CA-C    | 7.62  | 126.76      | 115.64   |
| 48  | R2    | 14  | ARG  | N-CA-C    | -7.62 | 99.99       | 110.35   |
| 48  | Y2    | 14  | ARG  | N-CA-C    | -7.61 | 100.00      | 110.35   |
| 54  | R8    | 38  | GLY  | N-CA-C    | -7.60 | 103.18      | 113.37   |
| 17  | QQ    | 57  | VAL  | N-CA-C    | 7.60  | 118.09      | 108.82   |
| 20  | XT    | 9   | ASN  | N-CA-C    | 7.59  | 121.72      | 110.48   |
| 40  | YU    | 70  | ARG  | N-CA-C    | -7.59 | 103.74      | 113.16   |
| 40  | RU    | 70  | ARG  | N-CA-C    | -7.59 | 103.74      | 113.16   |
| 33  | YN    | 116 | LEU  | N-CA-C    | -7.59 | 102.67      | 112.23   |
| 52  | R6    | 28  | ARG  | N-CA-C    | 7.57  | 120.37      | 108.79   |
| 27  | YD    | 251 | GLY  | N-CA-C    | 7.57  | 126.69      | 115.64   |
| 48  | Y2    | 21  | LEU  | N-CA-C    | -7.57 | 102.97      | 111.07   |
| 31  | RH    | 157 | TYR  | N-CA-C    | -7.55 | 103.14      | 112.88   |
| 31  | YH    | 157 | TYR  | N-CA-C    | -7.54 | 103.15      | 112.88   |
| 33  | RN    | 116 | LEU  | N-CA-C    | -7.54 | 102.73      | 112.23   |
| 28  | RE    | 185 | LYS  | N-CA-C    | 7.52  | 119.84      | 109.54   |
| 12  | QL    | 58  | VAL  | N-CA-C    | 7.51  | 118.89      | 107.77   |
| 28  | YE    | 185 | LYS  | N-CA-C    | 7.51  | 119.83      | 109.54   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 35  | YP    | 26  | GLY  | N-CA-C | -7.50 | 98.58       | 111.47   |
| 12  | XL    | 58  | VAL  | N-CA-C | 7.46  | 118.82      | 107.77   |
| 5   | XE    | 11  | ILE  | N-CA-C | 7.46  | 117.94      | 111.90   |
| 48  | Y2    | 41  | ILE  | N-CA-C | -7.45 | 103.30      | 112.76   |
| 52  | Y6    | 28  | ARG  | N-CA-C | 7.45  | 120.39      | 109.07   |
| 31  | RH    | 117 | PRO  | N-CA-C | 7.45  | 119.78      | 110.70   |
| 35  | RP    | 26  | GLY  | N-CA-C | -7.45 | 98.66       | 111.47   |
| 5   | QE    | 11  | ILE  | N-CA-C | 7.42  | 117.91      | 111.90   |
| 48  | R2    | 21  | LEU  | N-CA-C | -7.40 | 103.15      | 111.07   |
| 48  | R2    | 41  | ILE  | N-CA-C | -7.40 | 103.37      | 112.76   |
| 31  | YH    | 117 | PRO  | N-CA-C | 7.40  | 119.72      | 110.70   |
| 43  | YX    | 81  | VAL  | N-CA-C | 7.38  | 119.70      | 108.71   |
| 16  | QP    | 68  | ASP  | N-CA-C | -7.34 | 102.28      | 112.12   |
| 54  | R8    | 54  | GLU  | N-CA-C | -7.33 | 102.45      | 111.33   |
| 17  | QQ    | 60  | ILE  | N-CA-C | 7.33  | 118.67      | 108.12   |
| 12  | QL    | 44  | THR  | CA-C-N | 7.31  | 128.98      | 119.84   |
| 12  | QL    | 44  | THR  | C-N-CA | 7.31  | 128.98      | 119.84   |
| 43  | RX    | 81  | VAL  | N-CA-C | 7.29  | 119.57      | 108.71   |
| 54  | Y8    | 54  | GLU  | N-CA-C | -7.29 | 102.51      | 111.33   |
| 27  | YD    | 43  | ARG  | N-CA-C | 7.29  | 122.02      | 113.20   |
| 40  | RU    | 76  | TYR  | N-CA-C | -7.27 | 102.38      | 111.11   |
| 17  | XQ    | 60  | ILE  | N-CA-C | 7.27  | 118.59      | 108.12   |
| 27  | RD    | 43  | ARG  | N-CA-C | 7.27  | 122.00      | 113.20   |
| 41  | RV    | 49  | THR  | CA-C-N | -7.26 | 110.77      | 119.84   |
| 41  | RV    | 49  | THR  | C-N-CA | -7.26 | 110.77      | 119.84   |
| 9   | XI    | 63  | ILE  | N-CA-C | 7.25  | 118.50      | 107.77   |
| 14  | XN    | 53  | LEU  | CA-C-N | 7.25  | 127.66      | 119.83   |
| 14  | XN    | 53  | LEU  | C-N-CA | 7.25  | 127.66      | 119.83   |
| 31  | RH    | 139 | GLN  | N-CA-C | -7.25 | 103.38      | 111.28   |
| 4   | XD    | 14  | ARG  | CA-C-N | -7.25 | 107.82      | 122.31   |
| 4   | XD    | 14  | ARG  | C-N-CA | -7.25 | 107.82      | 122.31   |
| 41  | YV    | 49  | THR  | CA-C-N | -7.25 | 110.78      | 119.84   |
| 41  | YV    | 49  | THR  | C-N-CA | -7.25 | 110.78      | 119.84   |
| 40  | YU    | 76  | TYR  | N-CA-C | -7.22 | 102.44      | 111.11   |
| 27  | RD    | 53  | PHE  | N-CA-C | 7.21  | 121.66      | 112.86   |
| 9   | QI    | 63  | ILE  | N-CA-C | 7.21  | 118.44      | 107.77   |
| 48  | Y2    | 16  | LEU  | N-CA-C | -7.20 | 95.47       | 110.80   |
| 12  | XL    | 44  | THR  | CA-C-N | 7.20  | 128.84      | 119.84   |
| 12  | XL    | 44  | THR  | C-N-CA | 7.20  | 128.84      | 119.84   |
| 48  | R2    | 16  | LEU  | N-CA-C | -7.20 | 95.47       | 110.80   |
| 16  | XP    | 68  | ASP  | N-CA-C | -7.19 | 102.48      | 112.12   |
| 31  | YH    | 139 | GLN  | N-CA-C | -7.19 | 103.45      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 19  | XS    | 6   | LYS  | N-CA-C | -7.19 | 95.49       | 110.80   |
| 35  | YP    | 112 | LEU  | N-CA-C | 7.18  | 121.39      | 109.46   |
| 35  | RP    | 112 | LEU  | N-CA-C | 7.15  | 121.33      | 109.46   |
| 27  | YD    | 53  | PHE  | N-CA-C | 7.14  | 121.57      | 112.86   |
| 13  | QM    | 11  | ARG  | N-CA-C | 7.12  | 117.92      | 107.88   |
| 19  | QS    | 6   | LYS  | N-CA-C | -7.11 | 95.66       | 110.80   |
| 4   | XD    | 112 | VAL  | N-CA-C | 7.09  | 117.18      | 110.30   |
| 13  | XM    | 11  | ARG  | N-CA-C | 7.09  | 117.88      | 107.88   |
| 15  | QO    | 9   | GLN  | N-CA-C | -7.09 | 103.49      | 111.07   |
| 9   | XI    | 86  | VAL  | N-CA-C | -7.08 | 102.37      | 112.35   |
| 28  | YE    | 168 | MET  | N-CA-C | 7.08  | 121.06      | 109.94   |
| 28  | RE    | 168 | MET  | N-CA-C | 7.08  | 121.05      | 109.94   |
| 53  | Y7    | 19  | ARG  | N-CA-C | -7.07 | 103.62      | 111.82   |
| 9   | QI    | 86  | VAL  | N-CA-C | -7.07 | 102.39      | 112.35   |
| 29  | YF    | 203 | GLN  | N-CA-C | -7.06 | 103.28      | 110.97   |
| 4   | QD    | 112 | VAL  | N-CA-C | 7.05  | 117.14      | 110.30   |
| 14  | QN    | 53  | LEU  | CA-C-N | 7.05  | 127.44      | 119.83   |
| 14  | QN    | 53  | LEU  | C-N-CA | 7.05  | 127.44      | 119.83   |
| 29  | RF    | 203 | GLN  | N-CA-C | -7.03 | 103.31      | 110.97   |
| 53  | R7    | 19  | ARG  | N-CA-C | -7.03 | 103.67      | 111.82   |
| 19  | QS    | 36  | ARG  | N-CA-C | -6.98 | 104.73      | 113.18   |
| 15  | XO    | 9   | GLN  | N-CA-C | -6.97 | 103.61      | 111.07   |
| 18  | XR    | 50  | ILE  | N-CA-C | -6.97 | 100.58      | 109.58   |
| 34  | YO    | 90  | GLN  | N-CA-C | -6.96 | 104.40      | 113.17   |
| 39  | RT    | 80  | SER  | CA-C-N | 6.95  | 126.63      | 119.82   |
| 39  | RT    | 80  | SER  | C-N-CA | 6.95  | 126.63      | 119.82   |
| 28  | YE    | 188 | VAL  | CA-C-N | 6.95  | 128.52      | 119.84   |
| 28  | YE    | 188 | VAL  | C-N-CA | 6.95  | 128.52      | 119.84   |
| 19  | XS    | 36  | ARG  | N-CA-C | -6.94 | 104.79      | 113.18   |
| 36  | YQ    | 116 | GLU  | N-CA-C | -6.91 | 103.19      | 111.69   |
| 28  | RE    | 188 | VAL  | CA-C-N | 6.90  | 128.47      | 119.84   |
| 28  | RE    | 188 | VAL  | C-N-CA | 6.90  | 128.47      | 119.84   |
| 33  | YN    | 71  | ILE  | N-CA-C | 6.89  | 117.82      | 108.17   |
| 39  | YT    | 80  | SER  | CA-C-N | 6.89  | 126.57      | 119.82   |
| 39  | YT    | 80  | SER  | C-N-CA | 6.89  | 126.57      | 119.82   |
| 18  | QR    | 50  | ILE  | N-CA-C | -6.87 | 100.71      | 109.58   |
| 45  | RZ    | 157 | LEU  | CA-C-N | 6.87  | 127.45      | 120.38   |
| 45  | RZ    | 157 | LEU  | C-N-CA | 6.87  | 127.45      | 120.38   |
| 36  | RQ    | 116 | GLU  | N-CA-C | -6.86 | 103.25      | 111.69   |
| 42  | YW    | 9   | TYR  | N-CA-C | 6.86  | 120.97      | 112.47   |
| 40  | RU    | 81  | HIS  | N-CA-C | -6.86 | 103.73      | 111.07   |
| 29  | YF    | 24  | LEU  | CA-C-N | 6.86  | 128.41      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | YF    | 24  | LEU  | C-N-CA  | 6.86  | 128.41      | 119.84   |
| 36  | YQ    | 10  | ARG  | N-CA-C  | -6.85 | 99.14       | 110.17   |
| 34  | RO    | 90  | GLN  | N-CA-C  | -6.85 | 104.54      | 113.17   |
| 36  | RQ    | 10  | ARG  | N-CA-C  | -6.84 | 99.15       | 110.17   |
| 42  | RW    | 9   | TYR  | N-CA-C  | 6.84  | 120.96      | 112.47   |
| 38  | YS    | 110 | LEU  | N-CA-C  | 6.84  | 120.10      | 108.67   |
| 29  | RF    | 24  | LEU  | CA-C-N  | 6.82  | 128.37      | 119.84   |
| 29  | RF    | 24  | LEU  | C-N-CA  | 6.82  | 128.37      | 119.84   |
| 35  | RP    | 25  | SER  | N-CA-C  | -6.81 | 96.29       | 110.80   |
| 33  | RN    | 71  | ILE  | N-CA-C  | 6.80  | 117.70      | 108.17   |
| 38  | RS    | 110 | LEU  | N-CA-C  | 6.80  | 120.03      | 108.67   |
| 12  | XL    | 48  | PRO  | CA-N-CD | -6.79 | 102.50      | 112.00   |
| 35  | YP    | 25  | SER  | N-CA-C  | -6.78 | 96.37       | 110.80   |
| 6   | QF    | 60  | PHE  | N-CA-C  | 6.77  | 120.54      | 110.52   |
| 12  | QL    | 48  | PRO  | CA-N-CD | -6.76 | 102.54      | 112.00   |
| 36  | YQ    | 46  | GLN  | N-CA-C  | -6.75 | 105.05      | 113.55   |
| 40  | YU    | 81  | HIS  | N-CA-C  | -6.73 | 103.87      | 111.07   |
| 27  | RD    | 223 | GLY  | N-CA-C  | -6.73 | 104.35      | 112.49   |
| 6   | XF    | 60  | PHE  | N-CA-C  | 6.73  | 120.47      | 110.52   |
| 36  | RQ    | 46  | GLN  | N-CA-C  | -6.72 | 105.09      | 113.55   |
| 5   | XE    | 99  | GLY  | N-CA-C  | -6.70 | 102.18      | 111.76   |
| 39  | YT    | 111 | ARG  | N-CA-C  | -6.70 | 99.34       | 109.79   |
| 18  | QR    | 87  | ARG  | N-CA-C  | 6.69  | 118.74      | 110.91   |
| 18  | XR    | 87  | ARG  | N-CA-C  | 6.69  | 118.73      | 110.91   |
| 17  | QQ    | 62  | SER  | N-CA-C  | 6.68  | 116.87      | 108.45   |
| 5   | QE    | 99  | GLY  | N-CA-C  | -6.68 | 102.21      | 111.76   |
| 27  | YD    | 198 | ASN  | N-CA-C  | -6.68 | 102.27      | 111.28   |
| 37  | YR    | 76  | VAL  | N-CA-C  | -6.68 | 102.70      | 111.05   |
| 27  | RD    | 198 | ASN  | N-CA-C  | -6.67 | 102.27      | 111.28   |
| 39  | RT    | 111 | ARG  | N-CA-C  | -6.67 | 99.39       | 109.79   |
| 37  | YR    | 74  | LYS  | N-CA-C  | -6.66 | 101.74      | 110.33   |
| 37  | RR    | 76  | VAL  | N-CA-C  | -6.65 | 102.73      | 111.05   |
| 52  | R6    | 11  | LEU  | N-CA-C  | 6.62  | 120.31      | 109.72   |
| 27  | YD    | 223 | GLY  | N-CA-C  | -6.62 | 104.48      | 112.49   |
| 38  | YS    | 15  | ARG  | N-CA-C  | -6.61 | 103.56      | 111.69   |
| 52  | Y6    | 11  | LEU  | N-CA-C  | 6.61  | 120.29      | 109.72   |
| 37  | RR    | 74  | LYS  | N-CA-C  | -6.61 | 101.81      | 110.33   |
| 28  | YE    | 95  | ILE  | N-CA-C  | -6.60 | 104.42      | 113.00   |
| 36  | YQ    | 65  | PHE  | N-CA-C  | 6.59  | 121.85      | 113.55   |
| 27  | YD    | 14  | ARG  | N-CA-C  | -6.58 | 104.30      | 112.72   |
| 36  | RQ    | 65  | PHE  | N-CA-C  | 6.58  | 121.83      | 113.55   |
| 38  | RS    | 15  | ARG  | N-CA-C  | -6.58 | 103.60      | 111.69   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | YE    | 125 | GLY  | CA-C-N  | 6.57  | 128.06      | 119.84   |
| 28  | YE    | 125 | GLY  | C-N-CA  | 6.57  | 128.06      | 119.84   |
| 14  | XN    | 7   | ILE  | N-CA-C  | -6.57 | 104.08      | 110.72   |
| 36  | RQ    | 82  | ARG  | N-CA-C  | 6.54  | 123.83      | 114.16   |
| 19  | XS    | 79  | THR  | N-CA-C  | -6.52 | 96.90       | 110.80   |
| 27  | RD    | 14  | ARG  | N-CA-C  | -6.52 | 104.38      | 112.72   |
| 40  | YU    | 89  | GLU  | N-CA-C  | -6.51 | 103.84      | 113.61   |
| 28  | RE    | 95  | ILE  | N-CA-C  | -6.51 | 104.54      | 113.00   |
| 47  | R1    | 83  | GLU  | N-CA-C  | 6.51  | 120.45      | 110.36   |
| 17  | XQ    | 62  | SER  | N-CA-C  | 6.51  | 116.65      | 108.45   |
| 42  | RW    | 112 | GLY  | N-CA-C  | -6.50 | 106.71      | 115.36   |
| 14  | QN    | 7   | ILE  | N-CA-C  | -6.50 | 104.16      | 110.72   |
| 36  | YQ    | 82  | ARG  | N-CA-C  | 6.50  | 123.78      | 114.16   |
| 39  | RT    | 131 | ALA  | N-CA-C  | -6.49 | 104.94      | 112.92   |
| 47  | Y1    | 83  | GLU  | N-CA-C  | 6.48  | 120.41      | 110.36   |
| 40  | RU    | 89  | GLU  | N-CA-C  | -6.48 | 103.89      | 113.61   |
| 42  | YW    | 112 | GLY  | N-CA-C  | -6.47 | 106.76      | 115.36   |
| 31  | YH    | 164 | TYR  | N-CA-C  | -6.46 | 100.72      | 110.28   |
| 31  | RH    | 164 | TYR  | N-CA-C  | -6.46 | 100.72      | 110.28   |
| 28  | RE    | 125 | GLY  | CA-C-N  | 6.46  | 127.91      | 119.84   |
| 28  | RE    | 125 | GLY  | C-N-CA  | 6.46  | 127.91      | 119.84   |
| 19  | QS    | 79  | THR  | N-CA-C  | -6.45 | 97.06       | 110.80   |
| 30  | YG    | 55  | LYS  | N-CA-C  | -6.43 | 102.89      | 111.96   |
| 39  | YT    | 113 | LYS  | N-CA-C  | -6.42 | 102.96      | 111.24   |
| 54  | Y8    | 48  | PHE  | N-CA-C  | 6.41  | 118.86      | 108.34   |
| 30  | RG    | 55  | LYS  | N-CA-C  | -6.40 | 102.94      | 111.96   |
| 39  | RT    | 113 | LYS  | N-CA-C  | -6.39 | 103.00      | 111.24   |
| 54  | R8    | 50  | LEU  | N-CA-C  | 6.37  | 118.88      | 108.55   |
| 27  | YD    | 83  | GLU  | N-CA-C  | 6.37  | 118.87      | 109.69   |
| 27  | RD    | 83  | GLU  | N-CA-C  | 6.37  | 118.86      | 109.69   |
| 4   | XD    | 12  | CYS  | N-CA-C  | -6.36 | 104.34      | 111.28   |
| 54  | R8    | 48  | PHE  | N-CA-C  | 6.36  | 118.77      | 108.34   |
| 40  | RU    | 65  | ILE  | CB-CA-C | -6.35 | 103.87      | 111.81   |
| 30  | RG    | 28  | VAL  | N-CA-C  | 6.35  | 117.86      | 110.62   |
| 40  | YU    | 65  | ILE  | CB-CA-C | -6.34 | 103.88      | 111.81   |
| 33  | RN    | 113 | GLY  | N-CA-C  | -6.34 | 105.12      | 112.73   |
| 30  | YG    | 28  | VAL  | N-CA-C  | 6.34  | 117.85      | 110.62   |
| 39  | YT    | 123 | GLN  | N-CA-C  | -6.34 | 97.30       | 110.80   |
| 54  | R8    | 23  | VAL  | N-CA-C  | 6.34  | 117.15      | 107.77   |
| 39  | RT    | 130 | ALA  | N-CA-C  | -6.33 | 106.14      | 114.31   |
| 36  | YQ    | 106 | VAL  | N-CA-C  | 6.33  | 116.26      | 108.53   |
| 36  | RQ    | 106 | VAL  | N-CA-C  | 6.32  | 116.24      | 108.53   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 54  | Y8    | 50  | LEU  | N-CA-C | 6.32  | 118.78      | 108.55   |
| 16  | XP    | 74  | LEU  | N-CA-C | -6.32 | 105.73      | 113.50   |
| 39  | RT    | 123 | GLN  | N-CA-C | -6.31 | 97.35       | 110.80   |
| 5   | XE    | 32  | VAL  | N-CA-C | 6.31  | 117.56      | 108.48   |
| 5   | QE    | 32  | VAL  | N-CA-C | 6.30  | 117.56      | 108.48   |
| 39  | YT    | 131 | ALA  | N-CA-C | -6.30 | 105.17      | 112.92   |
| 13  | XM    | 91  | ARG  | N-CA-C | -6.30 | 105.45      | 113.01   |
| 33  | YN    | 113 | GLY  | N-CA-C | -6.28 | 105.19      | 112.73   |
| 12  | XL    | 89  | ARG  | N-CA-C | 6.28  | 118.63      | 110.53   |
| 33  | RN    | 107 | LEU  | N-CA-C | -6.28 | 101.88      | 109.72   |
| 16  | QP    | 74  | LEU  | N-CA-C | -6.27 | 105.78      | 113.50   |
| 54  | Y8    | 23  | VAL  | N-CA-C | 6.27  | 117.05      | 107.77   |
| 39  | YT    | 130 | ALA  | N-CA-C | -6.27 | 106.22      | 114.31   |
| 35  | YP    | 63  | PRO  | N-CA-C | 6.25  | 120.92      | 112.48   |
| 13  | QM    | 91  | ARG  | N-CA-C | -6.25 | 105.51      | 113.01   |
| 4   | XD    | 21  | LEU  | N-CA-C | -6.25 | 104.97      | 112.59   |
| 33  | YN    | 107 | LEU  | N-CA-C | -6.25 | 101.91      | 109.72   |
| 4   | QD    | 21  | LEU  | N-CA-C | -6.23 | 104.99      | 112.59   |
| 9   | QI    | 60  | ASP  | N-CA-C | -6.23 | 99.94       | 109.65   |
| 9   | XI    | 60  | ASP  | N-CA-C | -6.22 | 99.95       | 109.65   |
| 27  | YD    | 272 | ALA  | N-CA-C | 6.20  | 124.01      | 110.80   |
| 35  | RP    | 63  | PRO  | N-CA-C | 6.20  | 120.85      | 112.48   |
| 27  | YD    | 226 | MET  | N-CA-C | 6.20  | 117.87      | 110.19   |
| 27  | RD    | 272 | ALA  | N-CA-C | 6.19  | 123.98      | 110.80   |
| 21  | XU    | 8   | THR  | N-CA-C | 6.19  | 116.73      | 108.38   |
| 21  | QU    | 8   | THR  | N-CA-C | 6.18  | 116.72      | 108.38   |
| 27  | RD    | 226 | MET  | N-CA-C | 6.18  | 117.85      | 110.19   |
| 50  | Y4    | 68  | ARG  | N-CA-C | 6.18  | 123.95      | 110.80   |
| 19  | QS    | 39  | THR  | N-CA-C | -6.17 | 102.83      | 108.75   |
| 50  | R4    | 68  | ARG  | N-CA-C | 6.17  | 123.93      | 110.80   |
| 27  | YD    | 69  | ARG  | N-CA-C | 6.17  | 120.80      | 113.28   |
| 30  | RG    | 44  | GLY  | N-CA-C | -6.17 | 105.11      | 113.37   |
| 37  | YR    | 24  | GLN  | N-CA-C | -6.17 | 104.48      | 111.14   |
| 14  | QN    | 39  | LEU  | CA-C-N | -6.16 | 112.07      | 122.92   |
| 14  | QN    | 39  | LEU  | C-N-CA | -6.16 | 112.07      | 122.92   |
| 27  | RD    | 88  | ARG  | N-CA-C | 6.16  | 117.60      | 108.60   |
| 4   | XD    | 31  | CYS  | N-CA-C | -6.16 | 97.68       | 110.80   |
| 4   | QD    | 41  | GLY  | N-CA-C | 6.16  | 120.44      | 112.68   |
| 33  | RN    | 57  | ALA  | N-CA-C | -6.15 | 100.54      | 109.59   |
| 19  | XS    | 39  | THR  | N-CA-C | -6.15 | 102.85      | 108.75   |
| 37  | RR    | 24  | GLN  | N-CA-C | -6.15 | 104.50      | 111.14   |
| 41  | RV    | 14  | VAL  | N-CA-C | 6.14  | 116.75      | 110.05   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 32  | YI    | 133  | HIS  | CA-C-N    | -6.14 | 113.36      | 119.93   |
| 32  | YI    | 133  | HIS  | C-N-CA    | -6.14 | 113.36      | 119.93   |
| 12  | QL    | 89   | ARG  | N-CA-C    | 6.14  | 118.45      | 110.53   |
| 31  | RH    | 127  | GLU  | N-CA-C    | -6.14 | 96.25       | 109.81   |
| 43  | RX    | 5    | TYR  | N-CA-C    | -6.14 | 106.06      | 112.93   |
| 42  | YW    | 92   | ARG  | N-CA-C    | 6.14  | 117.84      | 111.03   |
| 33  | YN    | 13   | TRP  | N-CA-C    | 6.13  | 118.61      | 109.59   |
| 31  | YH    | 127  | GLU  | N-CA-C    | -6.13 | 96.26       | 109.81   |
| 33  | YN    | 57   | ALA  | N-CA-C    | -6.13 | 100.58      | 109.59   |
| 25  | YA    | 1473 | G    | O3'-P-O5' | -6.13 | 94.80       | 104.00   |
| 30  | YG    | 44   | GLY  | N-CA-C    | -6.12 | 105.16      | 113.37   |
| 27  | RD    | 69   | ARG  | N-CA-C    | 6.12  | 120.75      | 113.28   |
| 36  | RQ    | 97   | VAL  | N-CA-C    | 6.11  | 117.10      | 108.36   |
| 43  | YX    | 5    | TYR  | N-CA-C    | -6.11 | 106.09      | 112.93   |
| 27  | YD    | 22   | SER  | N-CA-C    | -6.10 | 103.95      | 111.40   |
| 39  | YT    | 76   | PHE  | CA-C-N    | 6.10  | 127.47      | 119.84   |
| 39  | YT    | 76   | PHE  | C-N-CA    | 6.10  | 127.47      | 119.84   |
| 27  | RD    | 22   | SER  | N-CA-C    | -6.10 | 103.96      | 111.40   |
| 42  | RW    | 60   | ASN  | N-CA-C    | 6.10  | 123.79      | 110.80   |
| 4   | XD    | 41   | GLY  | N-CA-C    | 6.10  | 120.36      | 112.68   |
| 42  | YW    | 60   | ASN  | N-CA-C    | 6.09  | 123.77      | 110.80   |
| 35  | RP    | 58   | THR  | N-CA-C    | -6.09 | 102.98      | 110.65   |
| 39  | RT    | 76   | PHE  | CA-C-N    | 6.09  | 127.45      | 119.84   |
| 39  | RT    | 76   | PHE  | C-N-CA    | 6.09  | 127.45      | 119.84   |
| 2   | XB    | 37   | ASN  | N-CA-C    | -6.09 | 105.81      | 113.23   |
| 33  | RN    | 13   | TRP  | N-CA-C    | 6.08  | 118.53      | 109.59   |
| 45  | RZ    | 178  | GLU  | N-CA-C    | 6.08  | 116.11      | 108.45   |
| 37  | RR    | 2    | ARG  | N-CA-C    | -6.07 | 97.86       | 110.80   |
| 28  | YE    | 77   | ILE  | N-CA-C    | -6.06 | 103.56      | 112.04   |
| 27  | RD    | 230  | ASP  | N-CA-C    | 6.06  | 119.92      | 111.56   |
| 36  | YQ    | 96   | VAL  | N-CA-C    | 6.06  | 115.97      | 107.37   |
| 37  | YR    | 111  | LEU  | N-CA-C    | 6.05  | 119.42      | 110.46   |
| 2   | QB    | 37   | ASN  | N-CA-C    | -6.05 | 105.85      | 113.23   |
| 36  | RQ    | 96   | VAL  | N-CA-C    | 6.05  | 115.96      | 107.37   |
| 35  | YP    | 58   | THR  | N-CA-C    | -6.04 | 103.03      | 110.65   |
| 36  | YQ    | 97   | VAL  | N-CA-C    | 6.04  | 117.00      | 108.36   |
| 48  | Y2    | 45   | SER  | N-CA-C    | 6.04  | 118.25      | 109.07   |
| 8   | XH    | 28   | ALA  | N-CA-C    | 6.03  | 118.33      | 110.43   |
| 27  | YD    | 230  | ASP  | N-CA-C    | 6.02  | 119.87      | 111.56   |
| 27  | YD    | 88   | ARG  | N-CA-C    | 6.02  | 117.39      | 108.60   |
| 35  | YP    | 62   | LEU  | N-CA-C    | 6.01  | 115.87      | 108.11   |
| 27  | RD    | 107  | ALA  | N-CA-C    | 6.01  | 118.31      | 109.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 41  | YV    | 14  | VAL  | N-CA-C | 6.01  | 116.60      | 110.05   |
| 37  | YR    | 2   | ARG  | N-CA-C | -6.00 | 98.01       | 110.80   |
| 42  | RW    | 92  | ARG  | N-CA-C | 6.00  | 117.69      | 111.03   |
| 28  | YE    | 18  | ASP  | N-CA-C | -6.00 | 98.94       | 109.02   |
| 27  | YD    | 107 | ALA  | N-CA-C | 6.00  | 118.29      | 109.42   |
| 47  | Y1    | 51  | VAL  | N-CA-C | 6.00  | 117.11      | 108.48   |
| 20  | QT    | 42  | GLN  | N-CA-C | -5.99 | 105.93      | 113.18   |
| 54  | R8    | 60  | LEU  | N-CA-C | -5.99 | 104.10      | 112.25   |
| 29  | RF    | 183 | VAL  | N-CA-C | 5.99  | 117.45      | 110.62   |
| 4   | XD    | 204 | ILE  | N-CA-C | -5.99 | 105.88      | 111.45   |
| 47  | R1    | 51  | VAL  | N-CA-C | 5.98  | 117.09      | 108.48   |
| 37  | RR    | 111 | LEU  | N-CA-C | 5.98  | 119.30      | 110.46   |
| 28  | RE    | 77  | ILE  | N-CA-C | -5.97 | 103.68      | 112.04   |
| 28  | RE    | 18  | ASP  | N-CA-C | -5.97 | 98.99       | 109.02   |
| 41  | RV    | 69  | LYS  | N-CA-C | 5.97  | 119.02      | 110.24   |
| 50  | R4    | 56  | VAL  | N-CA-C | -5.97 | 108.04      | 113.71   |
| 27  | RD    | 106 | ILE  | N-CA-C | -5.97 | 101.84      | 109.30   |
| 4   | QD    | 204 | ILE  | N-CA-C | -5.96 | 105.91      | 111.45   |
| 20  | XT    | 42  | GLN  | N-CA-C | -5.95 | 105.98      | 113.18   |
| 54  | Y8    | 60  | LEU  | N-CA-C | -5.95 | 104.16      | 112.25   |
| 35  | YP    | 19  | VAL  | N-CA-C | 5.95  | 121.71      | 109.34   |
| 35  | RP    | 62  | LEU  | N-CA-C | 5.94  | 115.78      | 108.11   |
| 35  | RP    | 19  | VAL  | N-CA-C | 5.94  | 121.69      | 109.34   |
| 48  | R2    | 45  | SER  | N-CA-C | 5.94  | 118.10      | 109.07   |
| 11  | QK    | 75  | TYR  | N-CA-C | -5.93 | 106.28      | 112.93   |
| 47  | R1    | 56  | GLN  | N-CA-C | 5.93  | 119.89      | 109.80   |
| 45  | RZ    | 133 | ILE  | N-CA-C | 5.93  | 112.95      | 107.56   |
| 29  | YF    | 183 | VAL  | N-CA-C | 5.93  | 117.38      | 110.62   |
| 11  | XK    | 116 | HIS  | N-CA-C | -5.92 | 103.28      | 111.81   |
| 33  | RN    | 38  | HIS  | N-CA-C | -5.92 | 106.40      | 113.97   |
| 41  | YV    | 69  | LYS  | N-CA-C | 5.91  | 118.93      | 110.24   |
| 27  | YD    | 196 | VAL  | N-CA-C | 5.90  | 120.39      | 111.89   |
| 33  | YN    | 38  | HIS  | N-CA-C | -5.90 | 106.42      | 113.97   |
| 20  | QT    | 77  | ALA  | N-CA-C | -5.89 | 104.93      | 111.71   |
| 5   | QE    | 150 | ARG  | N-CA-C | -5.89 | 105.68      | 112.92   |
| 27  | RD    | 99  | ASP  | N-CA-C | -5.88 | 105.37      | 112.54   |
| 27  | YD    | 200 | ASP  | N-CA-C | -5.88 | 105.60      | 112.89   |
| 29  | RF    | 151 | SER  | N-CA-C | -5.87 | 106.09      | 113.20   |
| 31  | RH    | 125 | VAL  | C-N-CD | -5.87 | 107.69      | 120.60   |
| 47  | Y1    | 56  | GLN  | N-CA-C | 5.87  | 119.78      | 109.80   |
| 13  | QM    | 24  | GLY  | N-CA-C | -5.87 | 107.58      | 115.21   |
| 27  | YD    | 106 | ILE  | N-CA-C | -5.87 | 101.97      | 109.30   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 27  | RD    | 200 | ASP  | N-CA-C | -5.86 | 105.62      | 112.89   |
| 2   | XB    | 24  | TRP  | CA-C-O | 5.86  | 121.34      | 117.94   |
| 42  | YW    | 101 | SER  | N-CA-C | 5.86  | 119.23      | 110.14   |
| 31  | YH    | 4   | ILE  | N-CA-C | 5.86  | 117.20      | 108.23   |
| 50  | Y4    | 56  | VAL  | N-CA-C | -5.86 | 108.14      | 113.71   |
| 8   | QH    | 28  | ALA  | N-CA-C | 5.86  | 118.31      | 110.35   |
| 13  | XM    | 24  | GLY  | N-CA-C | -5.85 | 107.60      | 115.21   |
| 27  | YD    | 99  | ASP  | N-CA-C | -5.85 | 105.40      | 112.54   |
| 27  | RD    | 196 | VAL  | N-CA-C | 5.85  | 120.31      | 111.89   |
| 51  | R5    | 4   | HIS  | CA-C-N | -5.85 | 113.91      | 119.76   |
| 51  | R5    | 4   | HIS  | C-N-CA | -5.85 | 113.91      | 119.76   |
| 42  | RW    | 101 | SER  | N-CA-C | 5.84  | 119.20      | 110.14   |
| 31  | YH    | 125 | VAL  | C-N-CD | -5.84 | 107.74      | 120.60   |
| 29  | YF    | 85  | GLY  | N-CA-C | -5.84 | 107.59      | 115.36   |
| 51  | Y5    | 4   | HIS  | CA-C-N | -5.84 | 113.92      | 119.76   |
| 51  | Y5    | 4   | HIS  | C-N-CA | -5.84 | 113.92      | 119.76   |
| 20  | QT    | 91  | LEU  | N-CA-C | -5.84 | 106.32      | 113.50   |
| 11  | XK    | 75  | TYR  | N-CA-C | -5.83 | 106.39      | 112.93   |
| 20  | XT    | 77  | ALA  | N-CA-C | -5.83 | 105.01      | 111.71   |
| 14  | QN    | 39  | LEU  | N-CA-C | 5.83  | 117.45      | 109.18   |
| 28  | RE    | 118 | LYS  | N-CA-C | -5.83 | 98.39       | 110.80   |
| 31  | RH    | 4   | ILE  | N-CA-C | 5.83  | 117.14      | 108.23   |
| 29  | YF    | 151 | SER  | N-CA-C | -5.82 | 106.16      | 113.20   |
| 5   | XE    | 150 | ARG  | N-CA-C | -5.82 | 105.77      | 112.92   |
| 36  | RQ    | 81  | VAL  | CA-C-N | -5.81 | 111.22      | 120.70   |
| 36  | RQ    | 81  | VAL  | C-N-CA | -5.81 | 111.22      | 120.70   |
| 36  | YQ    | 81  | VAL  | CA-C-N | -5.81 | 111.22      | 120.70   |
| 36  | YQ    | 81  | VAL  | C-N-CA | -5.81 | 111.22      | 120.70   |
| 9   | QI    | 118 | LYS  | N-CA-C | 5.81  | 118.83      | 109.83   |
| 9   | XI    | 118 | LYS  | N-CA-C | 5.81  | 118.83      | 109.83   |
| 8   | QH    | 12  | ARG  | N-CA-C | -5.81 | 104.95      | 111.28   |
| 38  | RS    | 6   | ALA  | N-CA-C | -5.80 | 105.04      | 111.71   |
| 42  | RW    | 6   | ILE  | N-CA-C | 5.79  | 117.10      | 108.23   |
| 31  | RH    | 161 | GLY  | N-CA-C | 5.79  | 118.29      | 111.63   |
| 39  | RT    | 70  | VAL  | N-CA-C | 5.79  | 116.81      | 108.48   |
| 9   | QI    | 55  | ALA  | N-CA-C | -5.78 | 103.63      | 111.55   |
| 30  | RG    | 58  | GLN  | N-CA-C | -5.78 | 105.72      | 112.89   |
| 20  | XT    | 91  | LEU  | N-CA-C | -5.78 | 106.39      | 113.50   |
| 8   | XH    | 12  | ARG  | N-CA-C | -5.77 | 104.99      | 111.28   |
| 6   | QF    | 95  | GLU  | CA-C-N | 5.77  | 127.05      | 119.84   |
| 6   | QF    | 95  | GLU  | C-N-CA | 5.77  | 127.05      | 119.84   |
| 5   | XE    | 26  | PHE  | N-CA-C | 5.77  | 118.99      | 109.94   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | QK    | 116 | HIS  | N-CA-C  | -5.76 | 103.51      | 111.81   |
| 28  | YE    | 118 | LYS  | N-CA-C  | -5.76 | 98.52       | 110.80   |
| 30  | YG    | 58  | GLN  | N-CA-C  | -5.76 | 105.75      | 112.89   |
| 38  | YS    | 12  | PHE  | N-CA-C  | -5.76 | 98.53       | 110.80   |
| 38  | RS    | 12  | PHE  | N-CA-C  | -5.74 | 98.57       | 110.80   |
| 39  | RT    | 121 | ILE  | N-CA-C  | -5.74 | 104.74      | 111.00   |
| 30  | YG    | 20  | ILE  | N-CA-C  | -5.74 | 104.76      | 110.62   |
| 29  | RF    | 85  | GLY  | N-CA-C  | -5.74 | 107.72      | 115.36   |
| 50  | Y4    | 67  | TYR  | N-CA-C  | 5.74  | 118.57      | 109.50   |
| 17  | XQ    | 46  | ASP  | CA-C-N  | 5.73  | 127.00      | 119.84   |
| 17  | XQ    | 46  | ASP  | C-N-CA  | 5.73  | 127.00      | 119.84   |
| 39  | YT    | 108 | ARG  | N-CA-C  | -5.73 | 106.46      | 113.50   |
| 17  | QQ    | 46  | ASP  | CA-C-N  | 5.72  | 126.99      | 119.84   |
| 17  | QQ    | 46  | ASP  | C-N-CA  | 5.72  | 126.99      | 119.84   |
| 9   | XI    | 55  | ALA  | N-CA-C  | -5.72 | 103.71      | 111.55   |
| 31  | YH    | 161 | GLY  | N-CA-C  | 5.72  | 118.21      | 111.63   |
| 28  | YE    | 159 | HIS  | N-CA-C  | -5.71 | 101.95      | 110.23   |
| 42  | YW    | 6   | ILE  | N-CA-C  | 5.71  | 116.97      | 108.23   |
| 50  | R4    | 67  | TYR  | N-CA-C  | 5.71  | 118.51      | 109.50   |
| 2   | QB    | 56  | ARG  | N-CA-C  | -5.70 | 104.43      | 111.33   |
| 2   | QB    | 7   | VAL  | N-CA-C  | 5.70  | 118.36      | 108.90   |
| 39  | YT    | 70  | VAL  | N-CA-C  | 5.70  | 116.68      | 108.48   |
| 5   | QE    | 26  | PHE  | N-CA-C  | 5.70  | 118.88      | 109.94   |
| 28  | YE    | 49  | LEU  | N-CA-C  | 5.70  | 119.75      | 112.12   |
| 19  | XS    | 45  | VAL  | N-CA-C  | 5.69  | 121.18      | 109.34   |
| 39  | YT    | 121 | ILE  | N-CA-C  | -5.69 | 104.80      | 111.00   |
| 30  | RG    | 20  | ILE  | N-CA-C  | -5.68 | 104.82      | 110.62   |
| 2   | XB    | 7   | VAL  | N-CA-C  | 5.68  | 118.33      | 108.90   |
| 2   | XB    | 108 | ILE  | N-CA-C  | -5.68 | 104.40      | 110.36   |
| 28  | YE    | 198 | VAL  | N-CA-C  | 5.68  | 116.31      | 107.28   |
| 5   | QE    | 11  | ILE  | CB-CA-C | -5.67 | 105.85      | 111.30   |
| 42  | YW    | 13  | SER  | CA-C-N  | 5.67  | 126.93      | 119.84   |
| 42  | YW    | 13  | SER  | C-N-CA  | 5.67  | 126.93      | 119.84   |
| 38  | RS    | 72  | ALA  | N-CA-C  | -5.67 | 105.02      | 111.14   |
| 28  | YE    | 131 | ALA  | CB-CA-C | -5.67 | 110.05      | 116.63   |
| 13  | QM    | 40  | ASN  | CA-C-N  | 5.67  | 125.03      | 118.85   |
| 13  | QM    | 40  | ASN  | C-N-CA  | 5.67  | 125.03      | 118.85   |
| 35  | RP    | 123 | LEU  | N-CA-C  | 5.66  | 117.57      | 109.14   |
| 44  | RY    | 44  | ILE  | N-CA-C  | 5.65  | 116.32      | 108.23   |
| 38  | YS    | 6   | ALA  | N-CA-C  | -5.65 | 105.21      | 111.71   |
| 35  | YP    | 123 | LEU  | N-CA-C  | 5.65  | 117.56      | 109.14   |
| 27  | YD    | 120 | GLY  | CA-C-N  | 5.65  | 125.49      | 119.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | YD    | 120 | GLY  | C-N-CA  | 5.65  | 125.49      | 119.28   |
| 28  | RE    | 49  | LEU  | N-CA-C  | 5.64  | 119.67      | 112.12   |
| 27  | RD    | 120 | GLY  | CA-C-N  | 5.64  | 125.48      | 119.28   |
| 27  | RD    | 120 | GLY  | C-N-CA  | 5.64  | 125.48      | 119.28   |
| 11  | QK    | 120 | ARG  | N-CA-C  | -5.63 | 102.52      | 110.29   |
| 39  | RT    | 108 | ARG  | N-CA-C  | -5.63 | 106.58      | 113.50   |
| 42  | RW    | 13  | SER  | N-CA-C  | 5.63  | 119.63      | 109.44   |
| 9   | XI    | 87  | GLN  | N-CA-C  | -5.63 | 104.78      | 111.03   |
| 28  | RE    | 159 | HIS  | N-CA-C  | -5.63 | 102.07      | 110.23   |
| 29  | RF    | 97  | TYR  | N-CA-C  | 5.62  | 119.62      | 112.87   |
| 19  | QS    | 45  | VAL  | N-CA-C  | 5.62  | 121.03      | 109.34   |
| 27  | YD    | 268 | ARG  | N-CA-C  | 5.62  | 119.64      | 112.34   |
| 29  | YF    | 97  | TYR  | N-CA-C  | 5.62  | 119.61      | 112.87   |
| 9   | QI    | 87  | GLN  | N-CA-C  | -5.61 | 104.80      | 111.03   |
| 13  | QM    | 88  | ARG  | N-CA-C  | -5.61 | 106.14      | 112.87   |
| 6   | XF    | 95  | GLU  | CA-C-N  | 5.61  | 126.85      | 119.84   |
| 6   | XF    | 95  | GLU  | C-N-CA  | 5.61  | 126.85      | 119.84   |
| 28  | YE    | 174 | ASP  | N-CA-C  | 5.61  | 115.64      | 108.24   |
| 38  | YS    | 53  | SER  | N-CA-C  | -5.60 | 106.61      | 113.50   |
| 2   | QB    | 108 | ILE  | N-CA-C  | -5.60 | 104.48      | 110.36   |
| 5   | XE    | 11  | ILE  | CB-CA-C | -5.59 | 105.93      | 111.30   |
| 13  | XM    | 40  | ASN  | CA-C-N  | 5.59  | 124.94      | 118.85   |
| 13  | XM    | 40  | ASN  | C-N-CA  | 5.59  | 124.94      | 118.85   |
| 9   | QI    | 93  | ARG  | N-CA-C  | -5.59 | 106.62      | 113.50   |
| 38  | YS    | 72  | ALA  | N-CA-C  | -5.58 | 105.11      | 111.14   |
| 40  | YU    | 50  | ARG  | N-CA-C  | -5.58 | 105.10      | 111.07   |
| 44  | YY    | 44  | ILE  | N-CA-C  | 5.58  | 116.21      | 108.23   |
| 36  | YQ    | 26  | TYR  | N-CA-C  | 5.58  | 119.18      | 111.71   |
| 27  | YD    | 11  | PRO  | N-CA-C  | -5.58 | 102.25      | 111.11   |
| 36  | YQ    | 21  | THR  | N-CA-C  | 5.57  | 122.67      | 110.80   |
| 42  | YW    | 13  | SER  | N-CA-C  | 5.57  | 119.53      | 109.44   |
| 27  | RD    | 268 | ARG  | N-CA-C  | 5.57  | 119.58      | 112.34   |
| 2   | XB    | 56  | ARG  | N-CA-C  | -5.57 | 104.59      | 111.33   |
| 28  | RE    | 93  | VAL  | N-CA-C  | -5.57 | 97.76       | 109.34   |
| 31  | RH    | 38  | SER  | CA-C-N  | 5.56  | 125.23      | 119.56   |
| 31  | RH    | 38  | SER  | C-N-CA  | 5.56  | 125.23      | 119.56   |
| 15  | QO    | 54  | ARG  | N-CA-C  | -5.56 | 104.24      | 111.02   |
| 28  | RE    | 198 | VAL  | N-CA-C  | 5.55  | 116.11      | 107.28   |
| 42  | RW    | 13  | SER  | CA-C-N  | 5.55  | 126.78      | 119.84   |
| 42  | RW    | 13  | SER  | C-N-CA  | 5.55  | 126.78      | 119.84   |
| 50  | Y4    | 15  | ILE  | N-CA-C  | 5.55  | 118.12      | 108.90   |
| 50  | R4    | 15  | ILE  | N-CA-C  | 5.55  | 118.11      | 108.90   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | RS    | 53  | SER  | N-CA-C  | -5.55 | 106.68      | 113.50   |
| 29  | YF    | 46  | ARG  | N-CA-C  | 5.54  | 119.76      | 112.89   |
| 28  | RE    | 131 | ALA  | CB-CA-C | -5.54 | 110.21      | 116.63   |
| 13  | XM    | 88  | ARG  | N-CA-C  | -5.53 | 106.23      | 112.87   |
| 15  | XO    | 54  | ARG  | N-CA-C  | -5.53 | 104.27      | 111.02   |
| 28  | YE    | 93  | VAL  | N-CA-C  | -5.53 | 97.83       | 109.34   |
| 43  | RX    | 12  | VAL  | N-CA-C  | -5.53 | 101.69      | 109.21   |
| 27  | RD    | 146 | GLU  | N-CA-C  | -5.53 | 101.86      | 110.42   |
| 43  | YX    | 38  | GLU  | N-CA-C  | -5.53 | 106.70      | 113.50   |
| 16  | XP    | 20  | VAL  | N-CA-C  | 5.52  | 117.00      | 108.44   |
| 43  | YX    | 12  | VAL  | N-CA-C  | -5.51 | 101.71      | 109.21   |
| 28  | RE    | 87  | GLU  | N-CA-C  | -5.51 | 103.87      | 111.81   |
| 9   | XI    | 93  | ARG  | N-CA-C  | -5.51 | 106.72      | 113.50   |
| 2   | QB    | 86  | GLU  | N-CA-C  | -5.51 | 104.91      | 111.69   |
| 27  | RD    | 174 | ILE  | N-CA-C  | 5.51  | 116.81      | 109.37   |
| 27  | YD    | 146 | GLU  | N-CA-C  | -5.51 | 101.88      | 110.42   |
| 16  | QP    | 20  | VAL  | N-CA-C  | 5.51  | 116.97      | 108.44   |
| 43  | RX    | 38  | GLU  | N-CA-C  | -5.51 | 106.73      | 113.50   |
| 12  | XL    | 127 | GLU  | N-CA-C  | -5.51 | 105.77      | 113.37   |
| 27  | RD    | 11  | PRO  | N-CA-C  | -5.50 | 102.36      | 111.11   |
| 28  | YE    | 87  | GLU  | N-CA-C  | -5.50 | 103.88      | 111.81   |
| 38  | YS    | 101 | LEU  | N-CA-C  | -5.50 | 104.92      | 111.69   |
| 28  | RE    | 174 | ASP  | N-CA-C  | 5.49  | 115.48      | 108.24   |
| 29  | RF    | 46  | ARG  | N-CA-C  | 5.49  | 119.69      | 112.89   |
| 41  | YV    | 17  | GLY  | N-CA-C  | -5.48 | 106.09      | 115.08   |
| 27  | RD    | 65  | ILE  | N-CA-C  | 5.47  | 116.01      | 110.05   |
| 19  | XS    | 80  | TYR  | N-CA-C  | 5.47  | 119.72      | 112.72   |
| 36  | RQ    | 21  | THR  | N-CA-C  | 5.46  | 122.43      | 110.80   |
| 40  | RU    | 50  | ARG  | N-CA-C  | -5.46 | 105.23      | 111.07   |
| 2   | XB    | 86  | GLU  | N-CA-C  | -5.46 | 104.98      | 111.69   |
| 27  | YD    | 174 | ILE  | N-CA-C  | 5.45  | 116.73      | 109.37   |
| 3   | QC    | 88  | ARG  | N-CA-C  | -5.44 | 106.34      | 112.87   |
| 55  | R9    | 3   | VAL  | N-CA-C  | 5.44  | 116.32      | 108.48   |
| 38  | RS    | 101 | LEU  | N-CA-C  | -5.44 | 105.00      | 111.69   |
| 35  | RP    | 85  | LEU  | N-CA-C  | -5.43 | 106.33      | 113.12   |
| 36  | RQ    | 26  | TYR  | N-CA-C  | 5.42  | 118.97      | 111.71   |
| 29  | YF    | 78  | ILE  | CB-CA-C | -5.42 | 104.94      | 112.04   |
| 9   | XI    | 61  | ALA  | N-CA-C  | 5.41  | 116.63      | 108.46   |
| 9   | QI    | 61  | ALA  | N-CA-C  | 5.41  | 116.63      | 108.46   |
| 42  | RW    | 21  | VAL  | N-CA-C  | -5.41 | 105.89      | 112.76   |
| 29  | RF    | 169 | ASN  | N-CA-C  | 5.41  | 118.97      | 112.38   |
| 47  | R1    | 85  | LEU  | N-CA-C  | 5.41  | 117.92      | 108.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 41  | RV    | 17   | GLY  | N-CA-C      | -5.40 | 106.23      | 115.08   |
| 44  | RY    | 70   | SER  | N-CA-C      | -5.39 | 106.87      | 113.50   |
| 34  | YO    | 57   | VAL  | N-CA-C      | -5.39 | 101.77      | 108.89   |
| 47  | Y1    | 85   | LEU  | N-CA-C      | 5.39  | 117.89      | 108.52   |
| 33  | YN    | 92   | ALA  | N-CA-C      | 5.39  | 117.15      | 111.28   |
| 10  | XJ    | 66   | ARG  | N-CA-C      | 5.38  | 117.49      | 108.23   |
| 29  | YF    | 169  | ASN  | N-CA-C      | 5.38  | 118.95      | 112.38   |
| 19  | QS    | 80   | TYR  | N-CA-C      | 5.38  | 119.61      | 112.72   |
| 29  | RF    | 10   | PRO  | N-CA-C      | 5.38  | 119.04      | 110.21   |
| 27  | YD    | 65   | ILE  | N-CA-C      | 5.38  | 115.92      | 110.05   |
| 12  | QL    | 127  | GLU  | N-CA-C      | -5.38 | 105.95      | 113.37   |
| 10  | QJ    | 66   | ARG  | N-CA-C      | 5.38  | 117.48      | 108.23   |
| 29  | RF    | 78   | ILE  | CB-CA-C     | -5.38 | 105.00      | 112.04   |
| 3   | XC    | 88   | ARG  | N-CA-C      | -5.38 | 106.42      | 112.87   |
| 13  | XM    | 107  | ALA  | N-CA-C      | -5.38 | 107.37      | 114.04   |
| 28  | RE    | 2    | LYS  | N-CA-C      | 5.37  | 118.58      | 110.64   |
| 48  | R2    | 39   | ALA  | N-CA-C      | -5.37 | 106.69      | 113.18   |
| 40  | YU    | 99   | ALA  | N-CA-C      | -5.37 | 106.43      | 112.87   |
| 30  | RG    | 31   | VAL  | CA-C-N      | 5.36  | 126.54      | 119.84   |
| 30  | RG    | 31   | VAL  | C-N-CA      | 5.36  | 126.54      | 119.84   |
| 40  | RU    | 99   | ALA  | N-CA-C      | -5.35 | 106.45      | 112.87   |
| 4   | QD    | 174  | LEU  | N-CA-C      | 5.35  | 117.62      | 108.90   |
| 7   | XG    | 45   | ASP  | N-CA-C      | -5.35 | 104.90      | 111.75   |
| 25  | RA    | 2848 | G    | C2'-C3'-O3' | 5.34  | 117.52      | 109.50   |
| 35  | RP    | 133  | SER  | N-CA-C      | 5.34  | 116.91      | 111.14   |
| 4   | XD    | 174  | LEU  | N-CA-C      | 5.34  | 117.61      | 108.90   |
| 4   | XD    | 28   | SER  | CA-C-N      | -5.34 | 113.17      | 119.84   |
| 4   | XD    | 28   | SER  | C-N-CA      | -5.34 | 113.17      | 119.84   |
| 13  | QM    | 107  | ALA  | N-CA-C      | -5.34 | 107.42      | 114.04   |
| 39  | RT    | 28   | VAL  | N-CA-C      | 5.33  | 115.39      | 108.35   |
| 5   | XE    | 97   | GLY  | N-CA-C      | -5.33 | 107.67      | 115.72   |
| 42  | YW    | 21   | VAL  | N-CA-C      | -5.33 | 105.99      | 112.76   |
| 34  | RO    | 57   | VAL  | N-CA-C      | -5.33 | 101.85      | 108.89   |
| 30  | YG    | 31   | VAL  | CA-C-N      | 5.33  | 126.50      | 119.84   |
| 30  | YG    | 31   | VAL  | C-N-CA      | 5.33  | 126.50      | 119.84   |
| 31  | YH    | 28   | GLY  | CA-C-N      | 5.33  | 126.50      | 119.84   |
| 31  | YH    | 28   | GLY  | C-N-CA      | 5.33  | 126.50      | 119.84   |
| 33  | RN    | 92   | ALA  | N-CA-C      | 5.32  | 117.08      | 111.28   |
| 35  | YP    | 85   | LEU  | N-CA-C      | -5.32 | 106.47      | 113.12   |
| 45  | YZ    | 100  | VAL  | CA-C-N      | 5.32  | 125.26      | 119.78   |
| 45  | YZ    | 100  | VAL  | C-N-CA      | 5.32  | 125.26      | 119.78   |
| 39  | YT    | 28   | VAL  | N-CA-C      | 5.32  | 115.37      | 108.35   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | RP    | 132  | LYS  | N-CA-C      | -5.31 | 104.74      | 111.11   |
| 8   | XH    | 70   | GLN  | N-CA-C      | 5.30  | 118.10      | 109.24   |
| 50  | Y4    | 12   | ALA  | N-CA-C      | 5.30  | 114.84      | 107.73   |
| 25  | RA    | 1130 | U    | C2'-C3'-O3' | 5.30  | 117.45      | 109.50   |
| 27  | RD    | 240  | ALA  | CA-C-N      | -5.30 | 113.22      | 119.84   |
| 27  | RD    | 240  | ALA  | C-N-CA      | -5.30 | 113.22      | 119.84   |
| 27  | YD    | 98   | VAL  | N-CA-C      | -5.30 | 105.81      | 113.07   |
| 29  | YF    | 199  | TRP  | N-CA-C      | -5.30 | 105.45      | 112.34   |
| 5   | QE    | 97   | GLY  | N-CA-C      | -5.30 | 107.72      | 115.72   |
| 37  | RR    | 94   | TYR  | N-CA-C      | -5.30 | 106.85      | 113.15   |
| 31  | RH    | 28   | GLY  | CA-C-N      | 5.29  | 126.45      | 119.84   |
| 31  | RH    | 28   | GLY  | C-N-CA      | 5.29  | 126.45      | 119.84   |
| 44  | YY    | 70   | SER  | N-CA-C      | -5.29 | 107.00      | 113.50   |
| 29  | RF    | 199  | TRP  | N-CA-C      | -5.28 | 105.47      | 112.34   |
| 35  | YP    | 133  | SER  | N-CA-C      | 5.28  | 116.84      | 111.14   |
| 27  | YD    | 133  | LEU  | N-CA-C      | 5.28  | 117.72      | 111.33   |
| 32  | RI    | 133  | HIS  | CA-C-N      | -5.28 | 114.28      | 119.93   |
| 32  | RI    | 133  | HIS  | C-N-CA      | -5.28 | 114.28      | 119.93   |
| 4   | QD    | 176  | LEU  | N-CA-C      | 5.28  | 116.93      | 107.80   |
| 8   | QH    | 70   | GLN  | N-CA-C      | 5.28  | 118.05      | 109.24   |
| 28  | YE    | 80   | GLU  | N-CA-C      | -5.28 | 100.83      | 109.80   |
| 29  | YF    | 10   | PRO  | N-CA-C      | 5.28  | 118.86      | 110.21   |
| 48  | Y2    | 39   | ALA  | N-CA-C      | -5.28 | 106.80      | 113.18   |
| 11  | XK    | 120  | ARG  | N-CA-C      | -5.27 | 102.54      | 110.24   |
| 28  | YE    | 2    | LYS  | N-CA-C      | 5.27  | 118.44      | 110.64   |
| 42  | RW    | 96   | ILE  | N-CA-C      | -5.26 | 101.94      | 108.89   |
| 35  | YP    | 36   | LYS  | N-CA-C      | 5.26  | 122.01      | 110.80   |
| 31  | YH    | 38   | SER  | CA-C-N      | 5.26  | 124.92      | 119.56   |
| 31  | YH    | 38   | SER  | C-N-CA      | 5.26  | 124.92      | 119.56   |
| 32  | YI    | 14   | ASP  | N-CA-C      | 5.26  | 116.84      | 108.79   |
| 37  | YR    | 94   | TYR  | N-CA-C      | -5.26 | 106.89      | 113.15   |
| 35  | YP    | 132  | LYS  | N-CA-C      | -5.25 | 104.81      | 111.11   |
| 30  | YG    | 99   | MET  | N-CA-C      | -5.25 | 105.24      | 111.69   |
| 27  | YD    | 240  | ALA  | CA-C-N      | -5.25 | 113.28      | 119.84   |
| 27  | YD    | 240  | ALA  | C-N-CA      | -5.25 | 113.28      | 119.84   |
| 30  | RG    | 99   | MET  | N-CA-C      | -5.24 | 105.24      | 111.69   |
| 28  | YE    | 200  | GLU  | N-CA-C      | -5.24 | 101.99      | 110.32   |
| 55  | Y9    | 3    | VAL  | N-CA-C      | 5.24  | 116.02      | 108.48   |
| 35  | YP    | 149  | GLU  | N-CA-C      | 5.23  | 118.20      | 107.37   |
| 8   | QH    | 137  | VAL  | N-CA-C      | 5.23  | 117.28      | 108.81   |
| 50  | Y4    | 18   | CYS  | CB-CA-C     | -5.22 | 108.85      | 116.53   |
| 28  | RE    | 97   | LYS  | N-CA-C      | -5.22 | 103.10      | 110.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | QG    | 45   | ASP  | N-CA-C      | -5.22 | 105.07      | 111.75   |
| 35  | RP    | 36   | LYS  | N-CA-C      | 5.22  | 121.92      | 110.80   |
| 4   | QD    | 28   | SER  | CA-C-N      | -5.22 | 113.32      | 119.84   |
| 4   | QD    | 28   | SER  | C-N-CA      | -5.22 | 113.32      | 119.84   |
| 28  | RE    | 80   | GLU  | N-CA-C      | -5.22 | 100.93      | 109.80   |
| 35  | RP    | 149  | GLU  | N-CA-C      | 5.21  | 118.16      | 107.37   |
| 35  | RP    | 147  | LEU  | N-CA-C      | 5.21  | 118.12      | 109.94   |
| 13  | QM    | 75   | ALA  | N-CA-C      | -5.21 | 105.68      | 111.36   |
| 11  | XK    | 26   | ASN  | N-CA-C      | 5.21  | 119.79      | 113.38   |
| 28  | YE    | 97   | LYS  | N-CA-C      | -5.21 | 103.12      | 110.31   |
| 47  | R1    | 17   | SER  | N-CA-C      | -5.21 | 100.24      | 108.73   |
| 50  | Y4    | 38   | LYS  | N-CA-C      | -5.21 | 105.81      | 113.72   |
| 41  | YV    | 6    | LYS  | N-CA-C      | 5.21  | 118.58      | 107.70   |
| 4   | XD    | 176  | LEU  | N-CA-C      | 5.20  | 116.80      | 107.80   |
| 13  | XM    | 46   | LYS  | N-CA-C      | -5.20 | 106.08      | 112.90   |
| 50  | R4    | 12   | ALA  | N-CA-C      | 5.20  | 114.70      | 107.73   |
| 17  | XQ    | 71   | PHE  | N-CA-C      | 5.20  | 117.64      | 108.75   |
| 27  | RD    | 98   | VAL  | N-CA-C      | -5.20 | 105.95      | 113.07   |
| 35  | YP    | 147  | LEU  | N-CA-C      | 5.19  | 118.09      | 109.94   |
| 28  | YE    | 79   | ARG  | N-CA-C      | 5.19  | 121.86      | 110.80   |
| 28  | YE    | 80   | GLU  | CA-C-N      | -5.19 | 117.66      | 123.16   |
| 28  | YE    | 80   | GLU  | C-N-CA      | -5.19 | 117.66      | 123.16   |
| 28  | RE    | 200  | GLU  | N-CA-C      | -5.18 | 102.08      | 110.32   |
| 29  | RF    | 80   | ALA  | CA-C-N      | 5.18  | 125.48      | 119.47   |
| 29  | RF    | 80   | ALA  | C-N-CA      | 5.18  | 125.48      | 119.47   |
| 5   | QE    | 67   | VAL  | N-CA-C      | 5.18  | 115.03      | 107.88   |
| 25  | RA    | 1992 | G    | C2'-C3'-O3' | 5.18  | 117.27      | 109.50   |
| 43  | RX    | 35   | THR  | N-CA-C      | 5.18  | 117.68      | 109.24   |
| 42  | YW    | 96   | ILE  | N-CA-C      | -5.17 | 102.06      | 108.89   |
| 50  | R4    | 38   | LYS  | N-CA-C      | -5.17 | 105.86      | 113.72   |
| 5   | XE    | 90   | VAL  | N-CA-C      | 5.17  | 115.41      | 108.17   |
| 8   | XH    | 137  | VAL  | N-CA-C      | 5.17  | 117.19      | 108.81   |
| 41  | RV    | 6    | LYS  | N-CA-C      | 5.17  | 118.50      | 107.70   |
| 28  | YE    | 194  | GLY  | N-CA-C      | -5.17 | 105.93      | 112.54   |
| 47  | R1    | 72   | GLU  | N-CA-C      | -5.17 | 106.08      | 112.38   |
| 50  | R4    | 18   | CYS  | CB-CA-C     | -5.16 | 108.94      | 116.53   |
| 28  | YE    | 46   | ALA  | N-CA-C      | 5.16  | 114.64      | 107.73   |
| 47  | Y1    | 17   | SER  | N-CA-C      | -5.16 | 100.32      | 108.73   |
| 47  | Y1    | 72   | GLU  | N-CA-C      | -5.16 | 106.09      | 112.38   |
| 27  | RD    | 133  | LEU  | N-CA-C      | 5.15  | 117.56      | 111.33   |
| 28  | RE    | 79   | ARG  | N-CA-C      | 5.15  | 121.77      | 110.80   |
| 34  | YO    | 58   | VAL  | N-CA-C      | 5.15  | 117.45      | 108.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 13  | QM    | 46   | LYS  | N-CA-C    | -5.15 | 106.16      | 112.90   |
| 18  | QR    | 86   | VAL  | N-CA-C    | 5.14  | 116.94      | 108.97   |
| 42  | YW    | 103  | ILE  | N-CA-C    | 5.14  | 115.75      | 107.73   |
| 25  | YA    | 1473 | G    | P-O5'-C5' | -5.14 | 113.19      | 120.90   |
| 54  | R8    | 53   | PRO  | N-CA-C    | -5.13 | 101.89      | 112.47   |
| 43  | YX    | 35   | THR  | N-CA-C    | 5.13  | 117.61      | 109.24   |
| 18  | XR    | 86   | VAL  | N-CA-C    | 5.13  | 116.93      | 108.97   |
| 47  | R1    | 18   | ILE  | N-CA-C    | 5.13  | 114.97      | 107.37   |
| 28  | RE    | 194  | GLY  | N-CA-C    | -5.13 | 105.97      | 112.54   |
| 37  | RR    | 9    | LYS  | CA-C-N    | -5.13 | 115.92      | 122.79   |
| 37  | RR    | 9    | LYS  | C-N-CA    | -5.13 | 115.92      | 122.79   |
| 48  | R2    | 56   | GLN  | N-CA-C    | -5.13 | 105.69      | 111.28   |
| 44  | RY    | 40   | GLU  | N-CA-C    | -5.13 | 106.85      | 114.64   |
| 54  | Y8    | 53   | PRO  | N-CA-C    | -5.12 | 101.92      | 112.47   |
| 28  | RE    | 46   | ALA  | N-CA-C    | 5.12  | 114.59      | 107.73   |
| 5   | XE    | 67   | VAL  | N-CA-C    | 5.12  | 114.94      | 107.88   |
| 28  | RE    | 80   | GLU  | CA-C-N    | -5.12 | 117.73      | 123.16   |
| 28  | RE    | 80   | GLU  | C-N-CA    | -5.12 | 117.73      | 123.16   |
| 2   | XB    | 90   | MET  | CA-C-N    | 5.12  | 125.27      | 119.90   |
| 2   | XB    | 90   | MET  | C-N-CA    | 5.12  | 125.27      | 119.90   |
| 11  | QK    | 26   | ASN  | N-CA-C    | 5.11  | 119.66      | 113.38   |
| 35  | RP    | 45   | LEU  | N-CA-C    | 5.10  | 118.01      | 110.46   |
| 47  | Y1    | 18   | ILE  | N-CA-C    | 5.10  | 114.92      | 107.37   |
| 51  | Y5    | 30   | LEU  | N-CA-C    | 5.09  | 118.05      | 109.95   |
| 27  | RD    | 243  | GLY  | N-CA-C    | -5.09 | 107.77      | 114.95   |
| 17  | QQ    | 71   | PHE  | N-CA-C    | 5.09  | 117.45      | 108.75   |
| 34  | RO    | 58   | VAL  | N-CA-C    | 5.09  | 117.35      | 108.90   |
| 13  | XM    | 75   | ALA  | N-CA-C    | -5.09 | 105.81      | 111.36   |
| 36  | RQ    | 90   | VAL  | N-CA-C    | 5.08  | 119.91      | 109.34   |
| 2   | QB    | 144  | ARG  | N-CA-C    | -5.08 | 105.82      | 111.36   |
| 19  | XS    | 23   | ASN  | N-CA-C    | -5.08 | 104.69      | 111.24   |
| 48  | Y2    | 56   | GLN  | N-CA-C    | -5.08 | 105.74      | 111.28   |
| 27  | RD    | 136  | ILE  | CA-C-N    | 5.08  | 125.87      | 119.98   |
| 27  | RD    | 136  | ILE  | C-N-CA    | 5.08  | 125.87      | 119.98   |
| 37  | YR    | 9    | LYS  | CA-C-N    | -5.07 | 115.99      | 122.79   |
| 37  | YR    | 9    | LYS  | C-N-CA    | -5.07 | 115.99      | 122.79   |
| 42  | RW    | 30   | GLU  | N-CA-C    | -5.07 | 105.45      | 111.69   |
| 2   | XB    | 24   | TRP  | N-CA-C    | 5.07  | 112.94      | 108.78   |
| 36  | YQ    | 90   | VAL  | N-CA-C    | 5.07  | 119.89      | 109.34   |
| 45  | YZ    | 112  | ARG  | N-CA-C    | -5.06 | 103.81      | 110.43   |
| 33  | RN    | 59   | LYS  | N-CA-C    | -5.05 | 104.04      | 111.81   |
| 51  | R5    | 41   | PRO  | CA-C-N    | 5.05  | 126.15      | 119.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 51  | R5    | 41  | PRO  | C-N-CA      | 5.05  | 126.15      | 119.84   |
| 14  | XN    | 39  | LEU  | N-CA-C      | 5.05  | 117.34      | 109.52   |
| 42  | RW    | 103 | ILE  | N-CA-C      | 5.04  | 115.59      | 107.73   |
| 2   | QB    | 182 | ILE  | CA-C-N      | 5.04  | 126.14      | 119.84   |
| 2   | QB    | 182 | ILE  | C-N-CA      | 5.04  | 126.14      | 119.84   |
| 48  | R2    | 52  | ASP  | N-CA-C      | -5.04 | 105.68      | 111.07   |
| 51  | Y5    | 41  | PRO  | CA-C-N      | 5.04  | 126.14      | 119.84   |
| 51  | Y5    | 41  | PRO  | C-N-CA      | 5.04  | 126.14      | 119.84   |
| 19  | QS    | 23  | ASN  | N-CA-C      | -5.04 | 104.75      | 111.24   |
| 5   | QE    | 90  | VAL  | N-CA-C      | 5.03  | 115.22      | 108.17   |
| 31  | YH    | 92  | ILE  | N-CA-C      | 5.03  | 119.81      | 109.34   |
| 35  | YP    | 45  | LEU  | N-CA-C      | 5.03  | 117.91      | 110.46   |
| 39  | YT    | 63  | VAL  | N-CA-C      | 5.03  | 115.16      | 108.11   |
| 33  | YN    | 59  | LYS  | N-CA-C      | -5.03 | 104.07      | 111.81   |
| 9   | XI    | 124 | GLN  | N-CA-C      | 5.02  | 117.44      | 109.96   |
| 2   | QB    | 27  | LYS  | N-CA-C      | -5.02 | 106.94      | 113.16   |
| 20  | QT    | 37  | SER  | N-CA-C      | -5.01 | 105.83      | 112.34   |
| 8   | XH    | 66  | GLY  | CA-C-N      | 5.01  | 126.11      | 119.84   |
| 8   | XH    | 66  | GLY  | C-N-CA      | 5.01  | 126.11      | 119.84   |
| 25  | YA    | 752 | A    | C4'-C3'-O3' | 5.01  | 116.92      | 109.40   |
| 30  | RG    | 43  | LEU  | N-CA-C      | 5.01  | 117.28      | 108.56   |
| 30  | YG    | 40  | ASN  | N-CA-C      | 5.01  | 117.98      | 109.76   |
| 20  | QT    | 14  | LYS  | N-CA-C      | -5.01 | 105.10      | 111.11   |
| 27  | YD    | 243 | GLY  | N-CA-C      | -5.01 | 107.89      | 114.95   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | QA    | 32247 | 0        | 16278    | 540     | 0            |
| 1   | XA    | 32249 | 0        | 16279    | 564     | 0            |
| 2   | QB    | 1924  | 0        | 1975     | 303     | 0            |
| 2   | XB    | 1924  | 0        | 1975     | 307     | 0            |
| 3   | QC    | 1605  | 0        | 1668     | 211     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | XC    | 1605  | 0        | 1668     | 212     | 0            |
| 4   | QD    | 1703  | 0        | 1764     | 269     | 0            |
| 4   | XD    | 1703  | 0        | 1765     | 230     | 1            |
| 5   | QE    | 1155  | 0        | 1213     | 156     | 0            |
| 5   | XE    | 1155  | 0        | 1213     | 146     | 0            |
| 6   | QF    | 843   | 0        | 857      | 100     | 1            |
| 6   | XF    | 843   | 0        | 857      | 105     | 0            |
| 7   | QG    | 1257  | 0        | 1296     | 154     | 0            |
| 7   | XG    | 1257  | 0        | 1294     | 151     | 0            |
| 8   | QH    | 1116  | 0        | 1175     | 158     | 0            |
| 8   | XH    | 1116  | 0        | 1177     | 157     | 0            |
| 9   | QI    | 1010  | 0        | 1037     | 151     | 0            |
| 9   | XI    | 1010  | 0        | 1037     | 161     | 0            |
| 10  | QJ    | 801   | 0        | 849      | 151     | 0            |
| 10  | XJ    | 801   | 0        | 849      | 137     | 0            |
| 11  | QK    | 885   | 0        | 904      | 108     | 0            |
| 11  | XK    | 885   | 0        | 904      | 111     | 0            |
| 12  | QL    | 975   | 0        | 1062     | 110     | 0            |
| 12  | XL    | 975   | 0        | 1062     | 108     | 0            |
| 13  | QM    | 964   | 0        | 1034     | 159     | 0            |
| 13  | XM    | 964   | 0        | 1034     | 169     | 0            |
| 14  | QN    | 492   | 0        | 529      | 98      | 0            |
| 14  | XN    | 492   | 0        | 529      | 99      | 0            |
| 15  | QO    | 734   | 0        | 771      | 81      | 0            |
| 15  | XO    | 734   | 0        | 771      | 81      | 0            |
| 16  | QP    | 705   | 0        | 725      | 116     | 0            |
| 16  | XP    | 705   | 0        | 725      | 112     | 0            |
| 17  | QQ    | 834   | 0        | 904      | 85      | 0            |
| 17  | XQ    | 834   | 0        | 904      | 76      | 0            |
| 18  | QR    | 574   | 0        | 644      | 74      | 0            |
| 18  | XR    | 574   | 0        | 644      | 74      | 0            |
| 19  | QS    | 674   | 0        | 699      | 116     | 0            |
| 19  | XS    | 674   | 0        | 699      | 137     | 0            |
| 20  | QT    | 763   | 0        | 860      | 109     | 0            |
| 20  | XT    | 763   | 0        | 861      | 110     | 0            |
| 21  | QU    | 217   | 0        | 234      | 29      | 0            |
| 21  | XU    | 217   | 0        | 234      | 26      | 0            |
| 22  | QV    | 1644  | 0        | 836      | 35      | 0            |
| 22  | XV    | 1644  | 0        | 836      | 35      | 0            |
| 23  | QY    | 323   | 0        | 165      | 4       | 0            |
| 23  | XY    | 323   | 0        | 165      | 7       | 0            |
| 24  | QX    | 173   | 0        | 88       | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | XX    | 173   | 0        | 88       | 6       | 0            |
| 25  | RA    | 62071 | 0        | 31288    | 890     | 1            |
| 25  | YA    | 62091 | 0        | 31294    | 904     | 1            |
| 26  | RB    | 2573  | 0        | 1306     | 65      | 0            |
| 26  | YB    | 2573  | 0        | 1306     | 32      | 0            |
| 27  | RD    | 2115  | 0        | 2195     | 312     | 0            |
| 27  | YD    | 2115  | 0        | 2195     | 335     | 0            |
| 28  | RE    | 1568  | 0        | 1634     | 287     | 0            |
| 28  | YE    | 1568  | 0        | 1634     | 275     | 0            |
| 29  | RF    | 1585  | 0        | 1632     | 186     | 0            |
| 29  | YF    | 1585  | 0        | 1632     | 190     | 0            |
| 30  | RG    | 1474  | 0        | 1535     | 220     | 1            |
| 30  | YG    | 1474  | 0        | 1535     | 214     | 1            |
| 31  | RH    | 1307  | 0        | 1382     | 231     | 0            |
| 31  | YH    | 1307  | 0        | 1382     | 231     | 0            |
| 32  | RI    | 1136  | 0        | 1223     | 41      | 0            |
| 32  | YI    | 1136  | 0        | 1223     | 51      | 0            |
| 33  | RN    | 1104  | 0        | 1180     | 205     | 0            |
| 33  | YN    | 1104  | 0        | 1180     | 195     | 0            |
| 34  | RO    | 933   | 0        | 996      | 129     | 0            |
| 34  | YO    | 933   | 0        | 996      | 135     | 0            |
| 35  | RP    | 1145  | 0        | 1228     | 255     | 0            |
| 35  | YP    | 1145  | 0        | 1228     | 248     | 1            |
| 36  | RQ    | 1122  | 0        | 1179     | 160     | 0            |
| 36  | YQ    | 1122  | 0        | 1179     | 156     | 0            |
| 37  | RR    | 968   | 0        | 1033     | 117     | 0            |
| 37  | YR    | 968   | 0        | 1033     | 110     | 0            |
| 38  | RS    | 882   | 0        | 943      | 166     | 0            |
| 38  | YS    | 882   | 0        | 943      | 166     | 0            |
| 39  | RT    | 1141  | 0        | 1202     | 155     | 0            |
| 39  | YT    | 1141  | 0        | 1202     | 160     | 0            |
| 40  | RU    | 964   | 0        | 1022     | 142     | 0            |
| 40  | YU    | 964   | 0        | 1022     | 147     | 0            |
| 41  | RV    | 779   | 0        | 852      | 137     | 0            |
| 41  | YV    | 779   | 0        | 852      | 135     | 13           |
| 42  | RW    | 900   | 0        | 964      | 105     | 0            |
| 42  | YW    | 900   | 0        | 964      | 107     | 0            |
| 43  | RX    | 725   | 0        | 778      | 69      | 0            |
| 43  | YX    | 725   | 0        | 778      | 68      | 0            |
| 44  | RY    | 785   | 0        | 878      | 164     | 0            |
| 44  | YY    | 785   | 0        | 878      | 163     | 0            |
| 45  | RZ    | 1461  | 0        | 1493     | 56      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45  | YZ    | 1461  | 0        | 1493     | 39      | 0            |
| 46  | R0    | 648   | 0        | 672      | 21      | 0            |
| 46  | Y0    | 648   | 0        | 672      | 23      | 0            |
| 47  | R1    | 763   | 0        | 848      | 149     | 0            |
| 47  | Y1    | 763   | 0        | 848      | 141     | 0            |
| 48  | R2    | 581   | 0        | 629      | 83      | 0            |
| 48  | Y2    | 581   | 0        | 629      | 78      | 0            |
| 49  | R3    | 469   | 0        | 518      | 42      | 1            |
| 49  | Y3    | 469   | 0        | 518      | 45      | 0            |
| 50  | R4    | 581   | 0        | 574      | 154     | 0            |
| 50  | Y4    | 581   | 0        | 574      | 170     | 0            |
| 51  | R5    | 459   | 0        | 480      | 74      | 0            |
| 51  | Y5    | 459   | 0        | 480      | 78      | 13           |
| 52  | R6    | 424   | 0        | 450      | 93      | 0            |
| 52  | Y6    | 424   | 0        | 450      | 92      | 0            |
| 53  | R7    | 430   | 0        | 480      | 41      | 0            |
| 53  | Y7    | 430   | 0        | 480      | 45      | 0            |
| 54  | R8    | 517   | 0        | 582      | 106     | 0            |
| 54  | Y8    | 517   | 0        | 582      | 103     | 0            |
| 55  | R9    | 307   | 0        | 335      | 24      | 0            |
| 55  | Y9    | 307   | 0        | 335      | 22      | 0            |
| 56  | Z6    | 74    | 0        | 51       | 6       | 0            |
| 56  | Z8    | 74    | 0        | 51       | 7       | 0            |
| 57  | QA    | 65    | 0        | 0        | 0       | 0            |
| 57  | QF    | 1     | 0        | 0        | 0       | 0            |
| 57  | QH    | 1     | 0        | 0        | 0       | 0            |
| 57  | QM    | 1     | 0        | 0        | 0       | 0            |
| 57  | QV    | 1     | 0        | 0        | 0       | 0            |
| 57  | QX    | 1     | 0        | 0        | 0       | 0            |
| 57  | R0    | 1     | 0        | 0        | 0       | 0            |
| 57  | R5    | 1     | 0        | 0        | 0       | 0            |
| 57  | RA    | 241   | 0        | 0        | 0       | 0            |
| 57  | RB    | 2     | 0        | 0        | 0       | 0            |
| 57  | RD    | 1     | 0        | 0        | 0       | 0            |
| 57  | RE    | 2     | 0        | 0        | 0       | 0            |
| 57  | RF    | 1     | 0        | 0        | 0       | 0            |
| 57  | RR    | 2     | 0        | 0        | 0       | 0            |
| 57  | XA    | 74    | 0        | 0        | 0       | 0            |
| 57  | Y0    | 1     | 0        | 0        | 0       | 0            |
| 57  | Y5    | 1     | 0        | 0        | 0       | 0            |
| 57  | YA    | 268   | 0        | 0        | 0       | 0            |
| 57  | YB    | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | YE    | 1      | 0        | 0        | 0       | 0            |
| 57  | YP    | 2      | 0        | 0        | 0       | 0            |
| 58  | QA    | 42     | 0        | 45       | 0       | 0            |
| 58  | XA    | 42     | 0        | 45       | 1       | 0            |
| 59  | QD    | 1      | 0        | 0        | 0       | 0            |
| 59  | QN    | 1      | 0        | 0        | 0       | 0            |
| 59  | R9    | 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   | 292002 | 0        | 198357   | 14883   | 17           |

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 31.

All (14883) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:XN:32:SER:CB   | 14:XN:41:ARG:HB3  | 1.23                     | 1.55              |
| 14:XN:32:SER:HB3  | 14:XN:41:ARG:CB   | 1.28                     | 1.54              |
| 31:RH:127:GLU:CG  | 31:RH:128:PRO:HD3 | 1.36                     | 1.53              |
| 31:YH:127:GLU:CG  | 31:YH:128:PRO:HD3 | 1.35                     | 1.52              |
| 4:XD:22:LYS:CG    | 4:XD:26:CYS:SG    | 2.01                     | 1.49              |
| 10:QJ:49:VAL:HG21 | 14:QN:41:ARG:CB   | 1.49                     | 1.42              |
| 4:XD:22:LYS:HB2   | 4:XD:26:CYS:SG    | 1.58                     | 1.41              |
| 4:XD:22:LYS:CB    | 4:XD:26:CYS:SG    | 2.10                     | 1.40              |
| 10:QJ:49:VAL:CG2  | 14:QN:41:ARG:CB   | 2.04                     | 1.35              |
| 47:R1:81:LYS:HA   | 47:R1:81:LYS:NZ   | 1.42                     | 1.34              |
| 47:Y1:81:LYS:HA   | 47:Y1:81:LYS:NZ   | 1.42                     | 1.34              |
| 4:QD:22:LYS:HG3   | 4:QD:26:CYS:SG    | 1.70                     | 1.31              |
| 10:QJ:49:VAL:CG2  | 14:QN:41:ARG:HB2  | 1.62                     | 1.29              |
| 4:XD:22:LYS:HG3   | 4:XD:26:CYS:SG    | 1.64                     | 1.26              |
| 47:R1:81:LYS:HE2  | 47:R1:81:LYS:N    | 1.50                     | 1.26              |
| 47:Y1:81:LYS:HE2  | 47:Y1:81:LYS:N    | 1.50                     | 1.26              |
| 14:QN:25:VAL:HG23 | 14:QN:38:GLY:O    | 1.37                     | 1.25              |
| 14:XN:40:CYS:SG   | 14:XN:43:CYS:N    | 2.11                     | 1.23              |
| 36:RQ:59:ARG:O    | 36:RQ:60:ARG:HD2  | 1.38                     | 1.22              |
| 47:Y1:82:LEU:HD12 | 47:Y1:82:LEU:C    | 1.66                     | 1.21              |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:CD  | 1.69                     | 1.21              |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:CD  | 1.70                     | 1.20              |
| 31:YH:127:GLU:CB  | 31:YH:128:PRO:HD3 | 1.69                     | 1.20              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:127:GLU:CB   | 31:RH:128:PRO:HD3  | 1.69                     | 1.19              |
| 47:R1:82:LEU:C     | 47:R1:82:LEU:HD12  | 1.66                     | 1.18              |
| 44:RY:95:LYS:HB3   | 44:RY:100:ALA:HA   | 1.20                     | 1.17              |
| 2:QB:101:MET:HA    | 2:QB:108:ILE:HG13  | 1.25                     | 1.17              |
| 4:XD:12:CYS:HA     | 4:XD:19:LEU:CD2    | 1.75                     | 1.17              |
| 44:YY:76:CYS:HB3   | 44:YY:96:ILE:HD13  | 1.17                     | 1.16              |
| 44:YY:95:LYS:HB3   | 44:YY:100:ALA:HA   | 1.20                     | 1.16              |
| 31:RH:132:ARG:HB2  | 31:RH:132:ARG:HH11 | 1.10                     | 1.16              |
| 14:YN:42:ILE:O     | 14:YN:43:CYS:O     | 1.65                     | 1.14              |
| 25:RA:1542:G:O6    | 25:RA:1543:A:N6    | 1.80                     | 1.14              |
| 35:RP:50:ARG:HH21  | 35:RP:50:ARG:HB3   | 1.13                     | 1.14              |
| 10:QJ:49:VAL:CG2   | 14:QN:41:ARG:HB3   | 1.71                     | 1.14              |
| 10:QJ:6:ILE:HG22   | 10:QJ:98:ILE:HG13  | 1.30                     | 1.13              |
| 19:QS:41:VAL:HB    | 19:QS:42:PRO:HA    | 1.26                     | 1.13              |
| 2:XB:101:MET:HA    | 2:XB:108:ILE:HG13  | 1.25                     | 1.13              |
| 4:XD:11:LEU:HD22   | 4:XD:66:ARG:HD3    | 1.29                     | 1.13              |
| 4:QD:12:CYS:HA     | 4:QD:19:LEU:HD21   | 1.24                     | 1.12              |
| 14:YN:32:SER:CB    | 14:YN:41:ARG:CB    | 1.97                     | 1.12              |
| 35:YP:50:ARG:HH21  | 35:YP:50:ARG:HB3   | 1.13                     | 1.12              |
| 47:Y1:82:LEU:CD1   | 47:Y1:83:GLU:O     | 1.97                     | 1.12              |
| 33:RN:1:MET:HE1    | 40:RU:95:LEU:HD21  | 1.27                     | 1.12              |
| 47:R1:82:LEU:CD1   | 47:R1:83:GLU:O     | 1.97                     | 1.12              |
| 40:RU:8:VAL:HG23   | 40:RU:11:ARG:HH21  | 1.14                     | 1.11              |
| 28:YE:179:GLU:HB3  | 28:YE:181:LEU:HD23 | 1.32                     | 1.11              |
| 40:YU:8:VAL:HG23   | 40:YU:11:ARG:HH21  | 1.14                     | 1.11              |
| 29:RF:101:LEU:HD12 | 29:RF:102:PRO:HD2  | 1.21                     | 1.11              |
| 27:YD:44:ASN:HB2   | 27:YD:48:ARG:O     | 1.51                     | 1.11              |
| 31:YH:132:ARG:HB2  | 31:YH:132:ARG:HH11 | 1.10                     | 1.11              |
| 27:RD:44:ASN:HB2   | 27:RD:48:ARG:O     | 1.50                     | 1.11              |
| 47:R1:81:LYS:HZ3   | 47:R1:81:LYS:CA    | 1.63                     | 1.11              |
| 47:Y1:82:LEU:HD12  | 47:Y1:83:GLU:N     | 1.66                     | 1.11              |
| 28:RE:179:GLU:HB3  | 28:RE:181:LEU:HD23 | 1.32                     | 1.10              |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:HD2  | 1.22                     | 1.10              |
| 33:YN:1:MET:HE1    | 40:YU:95:LEU:HD21  | 1.27                     | 1.10              |
| 11:QK:17:GLY:HA3   | 11:QK:77:MET:HE1   | 1.33                     | 1.10              |
| 31:RH:86:GLU:HG3   | 31:RH:165:ALA:H    | 1.06                     | 1.10              |
| 44:RY:76:CYS:HB3   | 44:RY:96:ILE:HD13  | 1.17                     | 1.10              |
| 1:XA:1054:C:OP2    | 1:XA:1197:G:OP2    | 1.67                     | 1.10              |
| 28:YE:50:GLY:HA2   | 28:YE:77:ILE:HA    | 1.31                     | 1.10              |
| 4:QD:22:LYS:CG     | 4:QD:26:CYS:SG     | 2.38                     | 1.10              |
| 10:XJ:6:ILE:HG22   | 10:XJ:98:ILE:HG13  | 1.30                     | 1.08              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:134:ARG:H    | 33:YN:135:PRO:HD3  | 1.11                     | 1.08              |
| 3:QC:15:THR:HG23   | 3:QC:181:ASN:HA    | 1.35                     | 1.08              |
| 11:QK:79:SER:HB2   | 11:QK:106:LYS:HD2  | 1.35                     | 1.08              |
| 15:XO:87:ILE:HG22  | 15:XO:88:ARG:H     | 1.19                     | 1.08              |
| 31:YH:152:ARG:HG3  | 31:YH:153:LYS:HE2  | 1.33                     | 1.08              |
| 35:RP:19:VAL:HG22  | 35:RP:20:GLY:H     | 1.15                     | 1.08              |
| 19:XS:41:VAL:HB    | 19:XS:42:PRO:HA    | 1.26                     | 1.08              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:H    | 1.05                     | 1.08              |
| 47:R1:82:LEU:HD12  | 47:R1:83:GLU:N     | 1.66                     | 1.08              |
| 2:XB:80:ILE:HD11   | 2:XB:208:ILE:HG23  | 1.34                     | 1.08              |
| 3:XC:15:THR:HG23   | 3:XC:181:ASN:HA    | 1.35                     | 1.08              |
| 27:YD:131:LEU:HB2  | 27:YD:136:ILE:HD11 | 1.35                     | 1.08              |
| 27:RD:131:LEU:HB2  | 27:RD:136:ILE:HD11 | 1.35                     | 1.07              |
| 47:Y1:81:LYS:HZ3   | 47:Y1:81:LYS:CA    | 1.65                     | 1.07              |
| 35:RP:126:VAL:HG12 | 35:RP:147:LEU:HD21 | 1.30                     | 1.07              |
| 31:RH:152:ARG:HG3  | 31:RH:153:LYS:HE2  | 1.34                     | 1.07              |
| 35:YP:126:VAL:HG12 | 35:YP:147:LEU:HD21 | 1.30                     | 1.07              |
| 15:QO:87:ILE:HG22  | 15:QO:88:ARG:H     | 1.18                     | 1.07              |
| 28:RE:50:GLY:HA2   | 28:RE:77:ILE:HA    | 1.31                     | 1.07              |
| 50:R4:71:ARG:HH11  | 50:R4:71:ARG:HG3   | 1.13                     | 1.07              |
| 10:QJ:49:VAL:HG21  | 14:QN:41:ARG:HB3   | 1.24                     | 1.06              |
| 47:Y1:82:LEU:CD1   | 47:Y1:83:GLU:N     | 2.18                     | 1.06              |
| 10:QJ:49:VAL:CG1   | 14:QN:41:ARG:HD2   | 1.85                     | 1.06              |
| 35:RP:59:LEU:HA    | 35:RP:61:ARG:NH2   | 1.69                     | 1.06              |
| 31:YH:153:LYS:HB3  | 31:YH:154:PRO:HD2  | 1.07                     | 1.06              |
| 35:YP:59:LEU:HA    | 35:YP:61:ARG:NH2   | 1.69                     | 1.06              |
| 50:Y4:71:ARG:HG3   | 50:Y4:71:ARG:HH11  | 1.13                     | 1.06              |
| 54:Y8:52:LYS:H     | 54:Y8:53:PRO:CD    | 1.69                     | 1.06              |
| 28:RE:21:VAL:HB    | 28:RE:22:PRO:HB3   | 1.37                     | 1.06              |
| 28:RE:63:LEU:HD12  | 28:RE:64:LYS:H     | 1.18                     | 1.06              |
| 47:R1:82:LEU:CD1   | 47:R1:83:GLU:N     | 2.18                     | 1.06              |
| 11:QK:51:LYS:HA    | 11:QK:55:LYS:HD3   | 1.36                     | 1.06              |
| 29:RF:46:ARG:HH11  | 29:RF:46:ARG:HG2   | 1.20                     | 1.06              |
| 4:XD:12:CYS:HA     | 4:XD:19:LEU:HD21   | 1.08                     | 1.05              |
| 13:QM:88:ARG:HH11  | 13:QM:88:ARG:HB3   | 1.19                     | 1.05              |
| 28:YE:63:LEU:HD12  | 28:YE:64:LYS:H     | 1.18                     | 1.05              |
| 13:XM:88:ARG:HH11  | 13:XM:88:ARG:HB3   | 1.19                     | 1.05              |
| 28:YE:21:VAL:HB    | 28:YE:22:PRO:HB3   | 1.37                     | 1.05              |
| 35:YP:19:VAL:HG22  | 35:YP:20:GLY:H     | 1.15                     | 1.05              |
| 5:QE:11:ILE:HD11   | 5:QE:31:LEU:HD12   | 1.38                     | 1.05              |
| 13:QM:49:THR:HG22  | 13:QM:51:ALA:H     | 1.22                     | 1.05              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:RN:134:ARG:H   | 33:RN:135:PRO:HD3  | 1.11                     | 1.05              |
| 11:XK:51:LYS:HA   | 11:XK:55:LYS:HD3   | 1.36                     | 1.05              |
| 13:QM:3:ARG:HA    | 13:QM:9:ILE:HG21   | 1.35                     | 1.05              |
| 13:XM:3:ARG:HA    | 13:XM:9:ILE:HG21   | 1.34                     | 1.05              |
| 25:YA:518:G:H4'   | 42:YW:18:ARG:HH12  | 1.18                     | 1.05              |
| 2:QB:80:ILE:HD11  | 2:QB:208:ILE:HG23  | 1.34                     | 1.04              |
| 31:RH:127:GLU:CB  | 31:RH:128:PRO:CD   | 2.35                     | 1.04              |
| 40:RU:90:VAL:HG12 | 40:RU:91:ASP:H     | 1.18                     | 1.04              |
| 11:XK:79:SER:HB2  | 11:XK:106:LYS:HD2  | 1.35                     | 1.04              |
| 36:RQ:59:ARG:O    | 36:RQ:60:ARG:CD    | 2.05                     | 1.04              |
| 37:RR:67:LEU:HD13 | 37:RR:76:VAL:HG21  | 1.39                     | 1.04              |
| 41:YV:49:THR:HB   | 41:YV:50:PRO:HD2   | 1.39                     | 1.04              |
| 38:RS:106:ARG:HA  | 38:RS:110:LEU:HD11 | 1.39                     | 1.04              |
| 31:YH:127:GLU:CG  | 31:YH:128:PRO:CD   | 2.31                     | 1.04              |
| 38:YS:83:LYS:O    | 38:YS:109:GLY:HA3  | 1.56                     | 1.04              |
| 40:YU:90:VAL:HG12 | 40:YU:91:ASP:H     | 1.18                     | 1.04              |
| 2:QB:18:GLY:H     | 2:QB:42:ILE:HG22   | 1.21                     | 1.03              |
| 10:QJ:49:VAL:CG1  | 14:QN:41:ARG:HB2   | 1.88                     | 1.03              |
| 14:XN:22:THR:O    | 14:XN:23:ARG:HB2   | 1.56                     | 1.03              |
| 19:XS:5:LEU:HD11  | 50:Y4:66:SER:HB2   | 1.38                     | 1.03              |
| 38:YS:106:ARG:HA  | 38:YS:110:LEU:HD11 | 1.39                     | 1.03              |
| 2:QB:4:GLU:HG2    | 2:QB:5:ILE:H       | 1.19                     | 1.03              |
| 4:QD:12:CYS:HA    | 4:QD:19:LEU:CD2    | 1.87                     | 1.03              |
| 36:RQ:81:VAL:O    | 36:RQ:82:ARG:CD    | 2.06                     | 1.03              |
| 38:RS:83:LYS:O    | 38:RS:109:GLY:HA3  | 1.56                     | 1.03              |
| 8:XH:29:SER:HB3   | 8:XH:32:LYS:HG3    | 1.39                     | 1.03              |
| 27:RD:35:LYS:HG2  | 27:RD:64:ILE:N     | 1.72                     | 1.03              |
| 2:XB:4:GLU:HG2    | 2:XB:5:ILE:H       | 1.20                     | 1.03              |
| 31:YH:127:GLU:CB  | 31:YH:128:PRO:CD   | 2.35                     | 1.03              |
| 34:YO:53:LYS:HD2  | 34:YO:53:LYS:H     | 1.23                     | 1.03              |
| 36:RQ:80:GLU:O    | 36:RQ:81:VAL:HG13  | 1.59                     | 1.02              |
| 54:R8:52:LYS:H    | 54:R8:53:PRO:CD    | 1.69                     | 1.02              |
| 27:YD:35:LYS:HG2  | 27:YD:64:ILE:N     | 1.72                     | 1.02              |
| 4:QD:166:LYS:CD   | 27:YD:134:ARG:NH1  | 2.21                     | 1.02              |
| 11:XK:17:GLY:HA3  | 11:XK:77:MET:HE1   | 1.33                     | 1.02              |
| 36:YQ:65:PHE:O    | 36:YQ:66:ILE:HG12  | 1.59                     | 1.02              |
| 29:RF:67:GLN:O    | 29:RF:67:GLN:HG3   | 1.58                     | 1.02              |
| 1:XA:1123:A:H4'   | 10:XJ:36:GLY:HA3   | 1.41                     | 1.02              |
| 2:XB:18:GLY:H     | 2:XB:42:ILE:HG22   | 1.22                     | 1.02              |
| 29:YF:67:GLN:O    | 29:YF:68:LYS:HB2   | 1.56                     | 1.02              |
| 36:YQ:12:GLN:HG2  | 36:YQ:73:PRO:HD2   | 1.42                     | 1.02              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 36:YQ:81:VAL:O      | 36:YQ:82:ARG:CD   | 2.06                     | 1.02              |
| 29:RF:67:GLN:O      | 29:RF:68:LYS:HB2  | 1.56                     | 1.02              |
| 36:RQ:12:GLN:HG2    | 36:RQ:73:PRO:HD2  | 1.42                     | 1.02              |
| 29:YF:46:ARG:HH11   | 29:YF:46:ARG:HG2  | 1.20                     | 1.02              |
| 31:RH:153:LYS:HB3   | 31:RH:154:PRO:HD2 | 1.07                     | 1.02              |
| 34:RO:53:LYS:HD2    | 34:RO:53:LYS:H    | 1.23                     | 1.02              |
| 25:YA:2701:C:H3'    | 25:YA:2702:U:H5'' | 1.41                     | 1.02              |
| 5:XE:11:ILE:HD11    | 5:XE:31:LEU:HD12  | 1.38                     | 1.01              |
| 30:YG:13:GLU:O      | 30:YG:14:GLU:HB2  | 1.60                     | 1.01              |
| 13:XM:49:THR:HG22   | 13:XM:51:ALA:H    | 1.22                     | 1.01              |
| 44:YY:97:ARG:HH21   | 44:YY:98:VAL:HB   | 1.26                     | 1.01              |
| 7:QG:78:ARG:HG3     | 7:QG:79:ARG:H     | 1.24                     | 1.01              |
| 19:QS:41:VAL:HB     | 19:QS:42:PRO:CA   | 1.91                     | 1.01              |
| 29:RF:185:ASP:HA    | 29:RF:188:ARG:HD3 | 1.41                     | 1.01              |
| 29:YF:67:GLN:O      | 29:YF:67:GLN:HG3  | 1.58                     | 1.01              |
| 10:QJ:49:VAL:HG13   | 14:QN:41:ARG:CD   | 1.90                     | 1.01              |
| 2:XB:178:ARG:HH21   | 8:XH:74:PRO:HB3   | 1.24                     | 1.01              |
| 19:XS:41:VAL:HB     | 19:XS:42:PRO:CA   | 1.91                     | 1.01              |
| 38:RS:26:LEU:HD12   | 38:RS:39:ILE:HD11 | 1.40                     | 1.00              |
| 44:RY:97:ARG:HH21   | 44:RY:98:VAL:HB   | 1.25                     | 1.00              |
| 4:XD:30:LYS:C       | 4:XD:32:ALA:H     | 1.62                     | 1.00              |
| 25:YA:270(T):G:H5'' | 47:Y1:97:LEU:HD22 | 1.43                     | 1.00              |
| 37:YR:67:LEU:HD13   | 37:YR:76:VAL:HG21 | 1.39                     | 1.00              |
| 27:RD:227:ASN:HB3   | 27:RD:228:PRO:HD2 | 1.44                     | 1.00              |
| 41:RV:49:THR:HB     | 41:RV:50:PRO:HD2  | 1.39                     | 1.00              |
| 8:QH:29:SER:HB3     | 8:QH:32:LYS:HG3   | 1.39                     | 1.00              |
| 36:RQ:65:PHE:O      | 36:RQ:66:ILE:HG12 | 1.59                     | 1.00              |
| 36:RQ:81:VAL:O      | 36:RQ:82:ARG:NE   | 1.94                     | 1.00              |
| 50:R4:56:VAL:HA     | 50:R4:60:GLN:HB2  | 1.43                     | 1.00              |
| 33:YN:96:GLU:HG2    | 33:YN:97:ARG:H    | 1.26                     | 1.00              |
| 37:YR:54:LEU:HD23   | 37:YR:66:VAL:HG23 | 1.44                     | 1.00              |
| 52:Y6:7:ILE:HG13    | 52:Y6:8:LYS:H     | 1.25                     | 1.00              |
| 25:RA:2701:C:H3'    | 25:RA:2702:U:H5'' | 1.44                     | 1.00              |
| 48:R2:50:ILE:HD12   | 48:R2:51:ARG:N    | 1.76                     | 1.00              |
| 29:YF:185:ASP:HA    | 29:YF:188:ARG:HD3 | 1.41                     | 1.00              |
| 36:YQ:80:GLU:O      | 36:YQ:81:VAL:HG13 | 1.59                     | 1.00              |
| 41:YV:1:MET:HE2     | 41:YV:43:GLU:HG2  | 1.42                     | 1.00              |
| 12:QL:8:ASN:OD1     | 17:QQ:34:LYS:HE2  | 1.61                     | 1.00              |
| 31:YH:153:LYS:HB3   | 31:YH:154:PRO:CD  | 1.92                     | 0.99              |
| 31:RH:153:LYS:HB3   | 31:RH:154:PRO:CD  | 1.92                     | 0.99              |
| 25:YA:1050:A:H8     | 25:YA:2751:G:HO2' | 1.08                     | 0.99              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:26:LEU:HD12  | 38:YS:39:ILE:HD11 | 1.40                     | 0.99              |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:H   | 1.26                     | 0.99              |
| 31:RH:77:LYS:HZ3   | 31:RH:77:LYS:HB3  | 1.22                     | 0.99              |
| 38:RS:83:LYS:NZ    | 38:RS:109:GLY:HA2 | 1.78                     | 0.99              |
| 25:YA:2015:A:H1'   | 51:Y5:2:ALA:HA    | 1.44                     | 0.99              |
| 31:RH:127:GLU:CG   | 31:RH:128:PRO:CD  | 2.31                     | 0.99              |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:H   | 1.26                     | 0.99              |
| 48:Y2:50:ILE:HD12  | 48:Y2:51:ARG:N    | 1.76                     | 0.99              |
| 3:QC:95:THR:HG22   | 3:QC:96:GLY:H     | 1.27                     | 0.99              |
| 8:QH:23:SER:HA     | 8:QH:63:LEU:HD22  | 1.45                     | 0.99              |
| 35:YP:105:LEU:O    | 35:YP:106:LEU:HB2 | 1.60                     | 0.99              |
| 8:QH:84:ARG:HH12   | 8:QH:86:ILE:HD13  | 1.28                     | 0.99              |
| 10:QJ:6:ILE:HD11   | 10:QJ:72:VAL:HB   | 1.44                     | 0.99              |
| 36:YQ:81:VAL:O     | 36:YQ:82:ARG:NE   | 1.94                     | 0.99              |
| 35:RP:50:ARG:HH21  | 35:RP:50:ARG:CB   | 1.76                     | 0.98              |
| 10:XJ:6:ILE:HD11   | 10:XJ:72:VAL:HB   | 1.44                     | 0.98              |
| 3:QC:181:ASN:HD21  | 3:QC:204:LEU:HD12 | 1.27                     | 0.98              |
| 42:RW:86:LEU:HD12  | 42:RW:87:PRO:HD2  | 1.45                     | 0.98              |
| 35:YP:50:ARG:HH21  | 35:YP:50:ARG:CB   | 1.76                     | 0.98              |
| 35:RP:105:LEU:O    | 35:RP:106:LEU:HB2 | 1.61                     | 0.98              |
| 39:RT:11:GLU:CD    | 39:RT:11:GLU:H    | 1.71                     | 0.98              |
| 7:XG:78:ARG:HG3    | 7:XG:79:ARG:H     | 1.23                     | 0.98              |
| 2:QB:196:LEU:HD12  | 2:QB:197:VAL:HG23 | 1.45                     | 0.98              |
| 39:YT:11:GLU:CD    | 39:YT:11:GLU:H    | 1.71                     | 0.98              |
| 30:RG:13:GLU:O     | 30:RG:14:GLU:HB2  | 1.60                     | 0.98              |
| 36:RQ:79:LEU:O     | 36:RQ:79:LEU:HD22 | 1.64                     | 0.98              |
| 3:QC:19:GLU:HA     | 3:QC:54:ARG:HH12  | 1.29                     | 0.98              |
| 27:RD:44:ASN:HB3   | 27:RD:49:ILE:HA   | 1.45                     | 0.98              |
| 4:XD:20:TYR:CD2    | 4:XD:27:TYR:CE2   | 2.51                     | 0.98              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:N   | 1.79                     | 0.98              |
| 4:QD:94:LEU:H      | 4:QD:94:LEU:HD12  | 1.28                     | 0.98              |
| 8:XH:84:ARG:HH12   | 8:XH:86:ILE:HD13  | 1.28                     | 0.97              |
| 36:YQ:79:LEU:HD13  | 36:YQ:79:LEU:O    | 1.63                     | 0.97              |
| 52:Y6:41:PRO:HG2   | 52:Y6:45:LYS:H    | 1.29                     | 0.97              |
| 3:QC:16:ARG:HD2    | 3:QC:54:ARG:HH21  | 1.28                     | 0.97              |
| 39:YT:62:THR:HG22  | 39:YT:75:ILE:HG12 | 1.46                     | 0.97              |
| 48:Y2:50:ILE:HD12  | 48:Y2:51:ARG:H    | 1.24                     | 0.97              |
| 4:QD:29:PRO:HG2    | 4:QD:30:LYS:CD    | 1.94                     | 0.97              |
| 28:RE:20:ALA:O     | 28:RE:21:VAL:HG22 | 1.65                     | 0.97              |
| 27:YD:44:ASN:HB3   | 27:YD:49:ILE:HA   | 1.45                     | 0.97              |
| 3:XC:16:ARG:HB2    | 3:XC:16:ARG:HH11  | 1.30                     | 0.97              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:YQ:79:LEU:O     | 36:YQ:79:LEU:HD22 | 1.64                     | 0.97              |
| 38:YS:83:LYS:NZ    | 38:YS:109:GLY:HA2 | 1.78                     | 0.97              |
| 25:RA:2015:A:H1'   | 51:R5:2:ALA:HA    | 1.47                     | 0.97              |
| 3:XC:181:ASN:HD21  | 3:XC:204:LEU:HD12 | 1.27                     | 0.97              |
| 33:RN:96:GLU:HG2   | 33:RN:97:ARG:H    | 1.26                     | 0.97              |
| 7:XG:62:PHE:HA     | 7:XG:124:LEU:HD21 | 1.47                     | 0.97              |
| 48:R2:50:ILE:HD12  | 48:R2:51:ARG:H    | 1.24                     | 0.97              |
| 36:RQ:79:LEU:O     | 36:RQ:79:LEU:HD13 | 1.63                     | 0.96              |
| 52:R6:7:ILE:HG13   | 52:R6:8:LYS:H     | 1.25                     | 0.96              |
| 51:Y5:58:LEU:HD13  | 51:Y5:60:VAL:HG12 | 1.47                     | 0.96              |
| 10:QJ:49:VAL:HG22  | 14:QN:41:ARG:CB   | 1.92                     | 0.96              |
| 42:YW:86:LEU:HD12  | 42:YW:87:PRO:HD2  | 1.45                     | 0.96              |
| 41:RV:1:MET:HE2    | 41:RV:43:GLU:HG2  | 1.42                     | 0.96              |
| 8:XH:23:SER:HA     | 8:XH:63:LEU:HD22  | 1.45                     | 0.96              |
| 4:QD:30:LYS:HG3    | 4:QD:35:ARG:NE    | 1.80                     | 0.96              |
| 26:RB:55:U:H4'     | 30:RG:29:TRP:HE1  | 1.30                     | 0.96              |
| 2:XB:7:VAL:HG21    | 2:XB:217:ARG:HH11 | 1.31                     | 0.96              |
| 2:QB:7:VAL:HG21    | 2:QB:217:ARG:HH11 | 1.31                     | 0.96              |
| 2:QB:8:LYS:HD3     | 2:QB:8:LYS:H      | 1.30                     | 0.96              |
| 22:QV:76:A:O2'     | 56:Z6:76:PPU:N    | 1.98                     | 0.96              |
| 30:RG:112:PRO:HB3  | 50:R4:37:SER:HB2  | 1.47                     | 0.96              |
| 4:QD:30:LYS:CB     | 4:QD:35:ARG:HG3   | 1.96                     | 0.96              |
| 52:R6:47:THR:HG22  | 52:R6:48:VAL:HG12 | 1.46                     | 0.96              |
| 1:XA:1286:A:H5''   | 21:XU:26:LYS:HD2  | 1.45                     | 0.96              |
| 3:XC:19:GLU:HA     | 3:XC:54:ARG:HH12  | 1.29                     | 0.96              |
| 3:XC:95:THR:HG22   | 3:XC:96:GLY:H     | 1.27                     | 0.96              |
| 10:XJ:32:ALA:HB3   | 10:XJ:76:ASN:HB2  | 1.48                     | 0.96              |
| 44:YY:84:ARG:HH12  | 44:YY:97:ARG:HB2  | 1.28                     | 0.96              |
| 12:QL:10:LEU:HD13  | 17:QQ:32:TYR:CE2  | 1.99                     | 0.96              |
| 7:QG:62:PHE:HA     | 7:QG:124:LEU:HD21 | 1.47                     | 0.95              |
| 37:RR:54:LEU:HD23  | 37:RR:66:VAL:HG23 | 1.44                     | 0.95              |
| 28:YE:20:ALA:O     | 28:YE:21:VAL:HG22 | 1.65                     | 0.95              |
| 30:YG:112:PRO:HB3  | 50:Y4:37:SER:HB2  | 1.47                     | 0.95              |
| 10:QJ:75:ILE:HG13  | 10:QJ:76:ASN:H    | 1.30                     | 0.95              |
| 16:QP:4:ILE:HD11   | 16:QP:64:ALA:HB1  | 1.46                     | 0.95              |
| 1:XA:686:U:H1'     | 11:XK:42:TRP:HE1  | 1.28                     | 0.95              |
| 51:Y5:56:LYS:H     | 51:Y5:56:LYS:HD2  | 1.31                     | 0.95              |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:CD  | 1.96                     | 0.95              |
| 10:QJ:32:ALA:HB3   | 10:QJ:76:ASN:HB2  | 1.47                     | 0.95              |
| 44:RY:84:ARG:HH12  | 44:RY:97:ARG:HB2  | 1.28                     | 0.95              |
| 12:QL:6:THR:H      | 12:QL:9:GLN:HE21  | 1.15                     | 0.95              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1473:G:O6    | 25:YA:1520:U:N3   | 1.99                     | 0.95              |
| 50:Y4:56:VAL:HA    | 50:Y4:60:GLN:HB2  | 1.44                     | 0.95              |
| 13:XM:57:ARG:HB2   | 13:XM:57:ARG:HH11 | 1.32                     | 0.95              |
| 4:QD:28:SER:HB2    | 4:QD:29:PRO:HD3   | 1.49                     | 0.95              |
| 3:XC:16:ARG:HD2    | 3:XC:54:ARG:HH21  | 1.28                     | 0.95              |
| 29:YF:103:LYS:HA   | 29:YF:106:ARG:HG3 | 1.48                     | 0.95              |
| 41:YV:99:ILE:HD13  | 41:YV:99:ILE:H    | 1.32                     | 0.95              |
| 29:RF:101:LEU:HD12 | 29:RF:102:PRO:CD  | 1.96                     | 0.95              |
| 4:XD:22:LYS:CD     | 4:XD:26:CYS:SG    | 2.55                     | 0.95              |
| 4:XD:94:LEU:H      | 4:XD:94:LEU:HD12  | 1.28                     | 0.95              |
| 27:YD:227:ASN:HB3  | 27:YD:228:PRO:HD2 | 1.44                     | 0.95              |
| 35:YP:62:LEU:N     | 35:YP:62:LEU:HD22 | 1.82                     | 0.95              |
| 47:Y1:81:LYS:N     | 47:Y1:81:LYS:CE   | 2.30                     | 0.95              |
| 31:RH:86:GLU:HG3   | 31:RH:165:ALA:N   | 1.79                     | 0.95              |
| 6:XF:86:ARG:O      | 6:XF:87:ARG:HG2   | 1.66                     | 0.95              |
| 48:R2:13:ALA:HA    | 48:R2:16:LEU:HD23 | 1.48                     | 0.94              |
| 2:XB:196:LEU:HD12  | 2:XB:197:VAL:HG23 | 1.45                     | 0.94              |
| 16:XP:4:ILE:HD11   | 16:XP:64:ALA:HB1  | 1.46                     | 0.94              |
| 31:YH:153:LYS:CB   | 31:YH:154:PRO:HD2 | 1.98                     | 0.94              |
| 47:Y1:81:LYS:CA    | 47:Y1:81:LYS:CE   | 2.45                     | 0.94              |
| 35:RP:62:LEU:N     | 35:RP:62:LEU:HD22 | 1.81                     | 0.94              |
| 48:Y2:13:ALA:HA    | 48:Y2:16:LEU:HD23 | 1.48                     | 0.94              |
| 47:R1:81:LYS:CA    | 47:R1:81:LYS:CE   | 2.45                     | 0.94              |
| 28:YE:78:LEU:HG    | 28:YE:79:ARG:HE   | 1.31                     | 0.94              |
| 44:RY:51:VAL:HG13  | 44:RY:52:SER:H    | 1.31                     | 0.94              |
| 44:YY:51:VAL:HG13  | 44:YY:52:SER:H    | 1.31                     | 0.94              |
| 3:QC:16:ARG:HB2    | 3:QC:16:ARG:HH11  | 1.30                     | 0.94              |
| 6:QF:86:ARG:O      | 6:QF:87:ARG:HG2   | 1.66                     | 0.94              |
| 34:RO:2:ILE:HD11   | 34:RO:82:ASN:HD22 | 1.33                     | 0.94              |
| 3:XC:11:ARG:HB3    | 3:XC:15:THR:HB    | 1.48                     | 0.94              |
| 2:XB:8:LYS:HD3     | 2:XB:8:LYS:H      | 1.30                     | 0.94              |
| 10:XJ:75:ILE:HG13  | 10:XJ:76:ASN:H    | 1.31                     | 0.94              |
| 41:YV:35:LEU:HD21  | 41:YV:57:VAL:HG22 | 1.47                     | 0.94              |
| 27:RD:28:GLU:HB2   | 27:RD:29:PRO:CD   | 1.98                     | 0.94              |
| 13:XM:77:ASN:HA    | 50:Y4:71:ARG:NH2  | 1.83                     | 0.94              |
| 27:YD:28:GLU:HB2   | 27:YD:29:PRO:CD   | 1.98                     | 0.94              |
| 27:RD:108:PRO:HB3  | 27:RD:143:HIS:HE1 | 1.32                     | 0.94              |
| 39:RT:62:THR:HG22  | 39:RT:75:ILE:HG12 | 1.46                     | 0.94              |
| 41:RV:35:LEU:HD21  | 41:RV:57:VAL:HG22 | 1.47                     | 0.94              |
| 47:R1:81:LYS:N     | 47:R1:81:LYS:CE   | 2.30                     | 0.94              |
| 52:R6:41:PRO:HG2   | 52:R6:45:LYS:H    | 1.29                     | 0.94              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:YH:77:LYS:HB3    | 31:YH:77:LYS:NZ    | 1.82                     | 0.94              |
| 7:QG:15:ASP:HB3     | 7:QG:20:ASP:H      | 1.31                     | 0.94              |
| 13:QM:90:LEU:HA     | 13:QM:93:ARG:HD2   | 1.50                     | 0.94              |
| 43:RX:57:LEU:CD1    | 43:RX:78:LYS:HB2   | 1.98                     | 0.94              |
| 19:QS:69:HIS:CE1    | 50:R4:69:LYS:HE2   | 2.03                     | 0.93              |
| 28:RE:78:LEU:HG     | 28:RE:79:ARG:HE    | 1.31                     | 0.93              |
| 35:RP:1:MET:HE2     | 35:RP:5:ASP:HB3    | 1.50                     | 0.93              |
| 51:R5:56:LYS:H      | 51:R5:56:LYS:HD2   | 1.30                     | 0.93              |
| 31:YH:77:LYS:HB3    | 31:YH:77:LYS:HZ3   | 1.31                     | 0.93              |
| 19:QS:63:THR:HG23   | 19:QS:66:MET:HE3   | 1.50                     | 0.93              |
| 33:RN:134:ARG:H     | 33:RN:135:PRO:CD   | 1.81                     | 0.93              |
| 38:RS:59:LYS:HG2    | 38:RS:60:GLY:H     | 1.31                     | 0.93              |
| 1:XA:664:G:H22      | 1:XA:741:G:H1      | 1.14                     | 0.93              |
| 25:RA:2729:G:H1'    | 28:RE:187:ALA:HB2  | 1.51                     | 0.93              |
| 3:XC:70:VAL:HG12    | 3:XC:72:LYS:H      | 1.34                     | 0.93              |
| 31:YH:127:GLU:HB3   | 31:YH:128:PRO:CD   | 1.99                     | 0.93              |
| 52:Y6:47:THR:HG22   | 52:Y6:48:VAL:HG12  | 1.46                     | 0.93              |
| 13:QM:57:ARG:HB2    | 13:QM:57:ARG:HH11  | 1.32                     | 0.93              |
| 4:XD:12:CYS:CA      | 4:XD:19:LEU:HD21   | 1.98                     | 0.93              |
| 33:YN:134:ARG:H     | 33:YN:135:PRO:CD   | 1.81                     | 0.93              |
| 19:QS:40:ILE:HG12   | 19:QS:41:VAL:HG22  | 1.51                     | 0.93              |
| 20:QT:49:ALA:HB1    | 20:QT:99:LEU:HB2   | 1.51                     | 0.93              |
| 36:RQ:59:ARG:O      | 36:RQ:60:ARG:CG    | 2.17                     | 0.93              |
| 43:YX:57:LEU:CD1    | 43:YX:78:LYS:HB2   | 1.98                     | 0.93              |
| 1:QA:686:U:H1'      | 11:QK:42:TRP:HE1   | 1.31                     | 0.93              |
| 41:RV:99:ILE:HD13   | 41:RV:99:ILE:H     | 1.32                     | 0.93              |
| 6:XF:24:GLU:HA      | 6:XF:27:GLN:HG3    | 1.49                     | 0.93              |
| 14:XN:43:CYS:O      | 14:XN:45:ARG:N     | 2.01                     | 0.93              |
| 31:RH:127:GLU:HB3   | 31:RH:128:PRO:CD   | 1.99                     | 0.93              |
| 36:RQ:34:LEU:HD11   | 36:RQ:129:THR:HB   | 1.50                     | 0.93              |
| 51:R5:58:LEU:HD13   | 51:R5:60:VAL:HG12  | 1.48                     | 0.93              |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:HD22  | 1.50                     | 0.93              |
| 17:XQ:4:LYS:HE3     | 17:XQ:6:LEU:HD21   | 1.51                     | 0.93              |
| 35:YP:1:MET:HE2     | 35:YP:5:ASP:HB3    | 1.50                     | 0.93              |
| 19:XS:40:ILE:HG12   | 19:XS:41:VAL:HG22  | 1.51                     | 0.92              |
| 35:YP:65:ARG:HG3    | 35:YP:65:ARG:HH11  | 1.34                     | 0.92              |
| 19:QS:68:GLY:HA3    | 50:R4:68:ARG:HG2   | 1.50                     | 0.92              |
| 27:RD:147:LEU:HD13  | 27:RD:155:LEU:HD11 | 1.51                     | 0.92              |
| 5:XE:53:LEU:H       | 5:XE:53:LEU:HD12   | 1.34                     | 0.92              |
| 27:YD:108:PRO:HB3   | 27:YD:143:HIS:CE1  | 2.05                     | 0.92              |
| 27:YD:108:PRO:HB3   | 27:YD:143:HIS:HE1  | 1.32                     | 0.92              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:YR:33:ARG:NH2   | 51:Y5:55:ARG:HG2  | 1.85                     | 0.92              |
| 10:XJ:8:LEU:HD11   | 10:XJ:23:ILE:HD12 | 1.49                     | 0.92              |
| 28:YE:14:ILE:HG12  | 28:YE:15:PHE:H    | 1.33                     | 0.92              |
| 15:XO:82:ILE:HD11  | 15:XO:88:ARG:HG3  | 1.51                     | 0.92              |
| 27:RD:183:ARG:HH11 | 27:RD:183:ARG:HG2 | 1.34                     | 0.92              |
| 5:QE:53:LEU:H      | 5:QE:53:LEU:HD12  | 1.35                     | 0.92              |
| 8:QH:6:ILE:HB      | 8:QH:85:ARG:NH1   | 1.85                     | 0.92              |
| 29:RF:103:LYS:HA   | 29:RF:106:ARG:HG3 | 1.48                     | 0.92              |
| 14:XN:32:SER:CB    | 14:XN:41:ARG:HB2  | 2.00                     | 0.92              |
| 38:YS:59:LYS:HG2   | 38:YS:60:GLY:H    | 1.31                     | 0.92              |
| 30:RG:37:VAL:HG22  | 30:RG:159:VAL:HA  | 1.52                     | 0.92              |
| 14:XN:32:SER:OG    | 14:XN:41:ARG:HB2  | 1.70                     | 0.92              |
| 4:QD:30:LYS:HB3    | 4:QD:35:ARG:HG3   | 1.52                     | 0.92              |
| 25:RA:270(R):G:N3  | 47:R1:78:LYS:NZ   | 2.18                     | 0.92              |
| 7:XG:15:ASP:HB3    | 7:XG:20:ASP:H     | 1.31                     | 0.92              |
| 2:QB:32:ILE:HD11   | 2:QB:40:HIS:HB3   | 1.52                     | 0.92              |
| 27:RD:108:PRO:HB3  | 27:RD:143:HIS:CE1 | 2.05                     | 0.92              |
| 31:RH:153:LYS:CB   | 31:RH:154:PRO:HD2 | 1.97                     | 0.92              |
| 8:XH:6:ILE:HB      | 8:XH:85:ARG:NH1   | 1.85                     | 0.92              |
| 38:YS:67:ARG:NH1   | 38:YS:67:ARG:HB2  | 1.85                     | 0.92              |
| 6:QF:24:GLU:HA     | 6:QF:27:GLN:HG3   | 1.49                     | 0.91              |
| 47:R1:81:LYS:HA    | 47:R1:81:LYS:CE   | 2.00                     | 0.91              |
| 15:QO:82:ILE:HD11  | 15:QO:88:ARG:HG3  | 1.51                     | 0.91              |
| 41:RV:24:LYS:HA    | 41:RV:92:THR:HG23 | 1.52                     | 0.91              |
| 5:XE:101:ILE:HD11  | 5:XE:119:LEU:HD23 | 1.51                     | 0.91              |
| 4:QD:9:CYS:SG      | 4:QD:31:CYS:O     | 2.28                     | 0.91              |
| 3:XC:20:SER:HB2    | 3:XC:40:ARG:HH22  | 1.34                     | 0.91              |
| 36:YQ:34:LEU:HD11  | 36:YQ:129:THR:HB  | 1.50                     | 0.91              |
| 47:Y1:81:LYS:HA    | 47:Y1:81:LYS:CE   | 2.00                     | 0.91              |
| 47:Y1:82:LEU:C     | 47:Y1:82:LEU:CD1  | 2.41                     | 0.91              |
| 37:RR:33:ARG:NH2   | 51:R5:55:ARG:HG2  | 1.84                     | 0.91              |
| 3:QC:11:ARG:HB3    | 3:QC:15:THR:HB    | 1.48                     | 0.91              |
| 3:QC:20:SER:HB2    | 3:QC:40:ARG:HH22  | 1.33                     | 0.91              |
| 8:QH:6:ILE:HD12    | 8:QH:6:ILE:H      | 1.35                     | 0.91              |
| 17:QQ:4:LYS:HE3    | 17:QQ:6:LEU:HD21  | 1.51                     | 0.91              |
| 30:YG:37:VAL:HG22  | 30:YG:159:VAL:HA  | 1.52                     | 0.91              |
| 40:YU:92:ARG:HG2   | 40:YU:92:ARG:O    | 1.69                     | 0.91              |
| 2:QB:33:TYR:HB2    | 2:QB:43:ASP:HB2   | 1.53                     | 0.91              |
| 10:QJ:8:LEU:HD11   | 10:QJ:23:ILE:HD12 | 1.50                     | 0.91              |
| 2:XB:33:TYR:HB2    | 2:XB:43:ASP:HB2   | 1.53                     | 0.91              |
| 44:YY:30:VAL:HG22  | 44:YY:37:VAL:HG12 | 1.53                     | 0.91              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:101:ILE:HG13 | 30:RG:102:PHE:N    | 1.86                     | 0.91              |
| 31:RH:77:LYS:HB3   | 31:RH:77:LYS:NZ    | 1.82                     | 0.91              |
| 27:YD:10:THR:HG23  | 27:YD:13:ARG:HB3   | 1.51                     | 0.91              |
| 5:QE:100:VAL:HG22  | 5:QE:118:ILE:HG22  | 1.52                     | 0.91              |
| 5:QE:101:ILE:HD11  | 5:QE:119:LEU:HD23  | 1.52                     | 0.91              |
| 28:RE:14:ILE:HG12  | 28:RE:15:PHE:H     | 1.33                     | 0.91              |
| 2:QB:77:ALA:HB2    | 2:QB:211:ILE:HD13  | 1.53                     | 0.91              |
| 3:QC:70:VAL:HG12   | 3:QC:72:LYS:H      | 1.34                     | 0.91              |
| 4:QD:29:PRO:HG2    | 4:QD:30:LYS:CE     | 2.01                     | 0.91              |
| 29:RF:7:TYR:HB3    | 29:RF:21:ALA:HB1   | 1.53                     | 0.91              |
| 25:YA:674:G:H1'    | 29:YF:74:ARG:HD3   | 1.52                     | 0.91              |
| 4:QD:29:PRO:HG2    | 4:QD:30:LYS:HD3    | 1.49                     | 0.91              |
| 4:QD:170:VAL:HG22  | 4:QD:171:GLY:H     | 1.34                     | 0.91              |
| 4:XD:170:VAL:HG22  | 4:XD:171:GLY:H     | 1.35                     | 0.91              |
| 47:Y1:80:LEU:O     | 47:Y1:81:LYS:HB2   | 1.71                     | 0.91              |
| 34:YO:2:ILE:HD11   | 34:YO:82:ASN:HD22  | 1.33                     | 0.90              |
| 8:XH:6:ILE:H       | 8:XH:6:ILE:HD12    | 1.34                     | 0.90              |
| 13:XM:90:LEU:HA    | 13:XM:93:ARG:HD2   | 1.50                     | 0.90              |
| 20:XT:49:ALA:HB1   | 20:XT:99:LEU:HB2   | 1.51                     | 0.90              |
| 27:RD:10:THR:HG23  | 27:RD:13:ARG:HB3   | 1.51                     | 0.90              |
| 38:RS:67:ARG:NH1   | 38:RS:67:ARG:HB2   | 1.85                     | 0.90              |
| 11:XK:99:GLN:HG2   | 11:XK:105:VAL:HG21 | 1.53                     | 0.90              |
| 5:XE:100:VAL:HG22  | 5:XE:118:ILE:HG22  | 1.52                     | 0.90              |
| 41:YV:24:LYS:HA    | 41:YV:92:THR:HG23  | 1.52                     | 0.90              |
| 44:YY:38:ILE:HG22  | 44:YY:66:PRO:HA    | 1.54                     | 0.90              |
| 31:RH:4:ILE:HG13   | 31:RH:6:ARG:CZ     | 2.01                     | 0.90              |
| 19:XS:63:THR:HG23  | 19:XS:66:MET:HE3   | 1.51                     | 0.90              |
| 35:YP:106:LEU:O    | 35:YP:107:LYS:HB2  | 1.71                     | 0.90              |
| 41:YV:44:LYS:O     | 41:YV:46:VAL:HG12  | 1.72                     | 0.90              |
| 31:YH:26:VAL:HG13  | 31:YH:27:LYS:H     | 1.35                     | 0.90              |
| 35:RP:58:THR:O     | 35:RP:61:ARG:NE    | 2.05                     | 0.90              |
| 1:QA:1286:A:H5''   | 21:QU:26:LYS:HD2   | 1.53                     | 0.90              |
| 4:QD:13:ARG:CB     | 4:QD:33:MET:HE3    | 2.02                     | 0.90              |
| 48:R2:65:ASN:HB3   | 48:R2:69:ARG:HH12  | 1.34                     | 0.90              |
| 27:YD:147:LEU:HD13 | 27:YD:155:LEU:HD11 | 1.51                     | 0.90              |
| 31:YH:4:ILE:HG13   | 31:YH:6:ARG:CZ     | 2.01                     | 0.90              |
| 51:Y5:3:LYS:HA     | 51:Y5:3:LYS:HE3    | 1.54                     | 0.90              |
| 36:RQ:59:ARG:O     | 36:RQ:60:ARG:HG3   | 1.72                     | 0.90              |
| 42:YW:65:LEU:HD12  | 42:YW:68:ARG:HH11  | 1.36                     | 0.90              |
| 31:RH:26:VAL:HG13  | 31:RH:27:LYS:H     | 1.36                     | 0.89              |
| 14:YN:22:THR:O     | 14:YN:23:ARG:CB    | 2.16                     | 0.89              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1021:A:OP2   | 33:YN:65:LYS:NZ   | 2.04                     | 0.89              |
| 27:YD:69:ARG:HH21  | 27:YD:130:ALA:HB2 | 1.37                     | 0.89              |
| 48:Y2:65:ASN:HB3   | 48:Y2:69:ARG:HH12 | 1.34                     | 0.89              |
| 2:QB:7:VAL:HG21    | 2:QB:217:ARG:NH1  | 1.86                     | 0.89              |
| 31:RH:10:PRO:HD2   | 31:RH:50:VAL:O    | 1.72                     | 0.89              |
| 2:XB:7:VAL:HG21    | 2:XB:217:ARG:NH1  | 1.87                     | 0.89              |
| 27:RD:69:ARG:HH21  | 27:RD:130:ALA:HB2 | 1.37                     | 0.89              |
| 27:YD:44:ASN:HD22  | 27:YD:44:ASN:H    | 1.19                     | 0.89              |
| 19:XS:64:GLU:O     | 19:XS:67:VAL:HG23 | 1.73                     | 0.89              |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:HG2 | 1.34                     | 0.89              |
| 30:YG:116:ASP:O    | 30:YG:117:PHE:HB3 | 1.72                     | 0.89              |
| 54:Y8:52:LYS:H     | 54:Y8:53:PRO:HD3  | 1.35                     | 0.89              |
| 1:QA:954:G:H4'     | 13:QM:121:LYS:HG3 | 1.55                     | 0.89              |
| 40:RU:92:ARG:HG2   | 40:RU:92:ARG:O    | 1.69                     | 0.89              |
| 41:RV:44:LYS:O     | 41:RV:46:VAL:HG12 | 1.72                     | 0.89              |
| 35:YP:88:LEU:HD12  | 35:YP:95:VAL:HG11 | 1.52                     | 0.89              |
| 54:Y8:59:LYS:HB2   | 54:Y8:59:LYS:NZ   | 1.87                     | 0.89              |
| 19:QS:64:GLU:O     | 19:QS:67:VAL:HG23 | 1.73                     | 0.89              |
| 25:RA:518:G:H4'    | 42:RW:18:ARG:HH12 | 1.38                     | 0.89              |
| 44:RY:76:CYS:SG    | 44:RY:77:PRO:HD2  | 2.13                     | 0.89              |
| 51:R5:3:LYS:HA     | 51:R5:3:LYS:HE3   | 1.54                     | 0.89              |
| 2:XB:126:GLU:HG3   | 2:XB:129:GLU:HG3  | 1.54                     | 0.89              |
| 28:YE:63:LEU:HD12  | 28:YE:64:LYS:N    | 1.87                     | 0.89              |
| 54:R8:52:LYS:H     | 54:R8:53:PRO:HD3  | 1.35                     | 0.89              |
| 12:XL:6:THR:H      | 12:XL:9:GLN:HE21  | 1.15                     | 0.89              |
| 35:YP:58:THR:O     | 35:YP:61:ARG:NE   | 2.05                     | 0.89              |
| 10:QJ:74:ILE:H     | 10:QJ:74:ILE:HD13 | 1.38                     | 0.89              |
| 35:RP:65:ARG:HG3   | 35:RP:65:ARG:HH11 | 1.35                     | 0.89              |
| 1:XA:27:G:H4'      | 4:XD:209:ARG:HG3  | 1.52                     | 0.89              |
| 2:XB:32:ILE:HD11   | 2:XB:40:HIS:HB3   | 1.52                     | 0.89              |
| 25:YA:483:A:H4'    | 44:YY:49:VAL:HA   | 1.55                     | 0.89              |
| 30:YG:88:ILE:O     | 30:YG:88:ILE:HD13 | 1.72                     | 0.89              |
| 35:RP:88:LEU:HD12  | 35:RP:95:VAL:HG11 | 1.52                     | 0.89              |
| 2:QB:18:GLY:N      | 2:QB:42:ILE:HG22  | 1.86                     | 0.88              |
| 2:QB:126:GLU:HG3   | 2:QB:129:GLU:HG3  | 1.54                     | 0.88              |
| 47:R1:81:LYS:HA    | 47:R1:81:LYS:HZ3  | 0.75                     | 0.88              |
| 31:YH:10:PRO:HD2   | 31:YH:50:VAL:O    | 1.72                     | 0.88              |
| 51:Y5:40:LYS:HZ1   | 51:Y5:48:GLU:HB2  | 1.37                     | 0.88              |
| 5:QE:41:VAL:HG11   | 5:QE:113:ALA:HB2  | 1.54                     | 0.88              |
| 27:RD:27:THR:HG23  | 27:RD:28:GLU:H    | 1.38                     | 0.88              |
| 2:XB:77:ALA:HB2    | 2:XB:211:ILE:HD13 | 1.53                     | 0.88              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:RY:30:VAL:HG22 | 44:RY:37:VAL:HG12  | 1.53                     | 0.88              |
| 47:R1:80:LEU:O    | 47:R1:81:LYS:HB2   | 1.71                     | 0.88              |
| 25:YA:2712:U:HO2' | 25:YA:2712(A):A:H8 | 0.97                     | 0.88              |
| 35:YP:64:LYS:O    | 35:YP:66:GLY:N     | 2.06                     | 0.88              |
| 51:R5:40:LYS:HZ1  | 51:R5:48:GLU:HB2   | 1.38                     | 0.88              |
| 2:XB:18:GLY:N     | 2:XB:42:ILE:HG22   | 1.87                     | 0.88              |
| 5:XE:71:LEU:O     | 5:XE:72:GLN:HG3    | 1.74                     | 0.88              |
| 33:YN:22:THR:HG22 | 33:YN:23:LEU:N     | 1.88                     | 0.88              |
| 30:RG:88:ILE:HD13 | 30:RG:88:ILE:O     | 1.72                     | 0.88              |
| 35:RP:106:LEU:O   | 35:RP:107:LYS:HB2  | 1.71                     | 0.88              |
| 38:YS:106:ARG:NH1 | 38:YS:106:ARG:HB2  | 1.88                     | 0.88              |
| 44:YY:76:CYS:SG   | 44:YY:77:PRO:HD2   | 2.13                     | 0.88              |
| 14:XN:12:ARG:C    | 14:XN:14:PRO:HD2   | 1.98                     | 0.88              |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:N     | 1.88                     | 0.88              |
| 33:RN:22:THR:HG22 | 33:RN:23:LEU:N     | 1.88                     | 0.88              |
| 11:QK:99:GLN:HG2  | 11:QK:105:VAL:HG21 | 1.53                     | 0.88              |
| 13:QM:97:PRO:HB2  | 13:QM:101:GLN:NE2  | 1.89                     | 0.88              |
| 24:XX:2:U:O2'     | 24:XX:3:G:H5'      | 1.74                     | 0.88              |
| 8:QH:51:VAL:HG21  | 8:QH:60:ARG:HG2    | 1.55                     | 0.88              |
| 54:R8:59:LYS:HB2  | 54:R8:59:LYS:NZ    | 1.88                     | 0.88              |
| 20:XT:23:ARG:HA   | 20:XT:26:ASN:HD21  | 1.36                     | 0.88              |
| 1:QA:559:A:H4'    | 1:QA:560:U:H3'     | 1.56                     | 0.88              |
| 35:YP:49:ARG:HD2  | 54:Y8:58:ILE:HG22  | 1.54                     | 0.88              |
| 25:RA:2451:A:C6   | 56:Z6:76:PPU:HE2   | 2.09                     | 0.87              |
| 35:RP:49:ARG:HD2  | 54:R8:58:ILE:HG22  | 1.54                     | 0.87              |
| 38:RS:106:ARG:NH1 | 38:RS:106:ARG:HB2  | 1.88                     | 0.87              |
| 41:RV:19:LYS:HD2  | 41:RV:95:LEU:HD23  | 1.55                     | 0.87              |
| 44:RY:38:ILE:HG22 | 44:RY:66:PRO:HA    | 1.54                     | 0.87              |
| 4:XD:114:ARG:HH11 | 4:XD:114:ARG:HG3   | 1.38                     | 0.87              |
| 5:XE:41:VAL:HG11  | 5:XE:113:ALA:HB2   | 1.54                     | 0.87              |
| 27:YD:27:THR:HG23 | 27:YD:28:GLU:H     | 1.38                     | 0.87              |
| 27:YD:44:ASN:CB   | 27:YD:49:ILE:HA    | 2.04                     | 0.87              |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:N     | 1.89                     | 0.87              |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:N     | 1.89                     | 0.87              |
| 42:RW:65:LEU:HD12 | 42:RW:68:ARG:HH11  | 1.36                     | 0.87              |
| 21:XU:6:ARG:HE    | 21:XU:15:ARG:CZ    | 1.87                     | 0.87              |
| 19:QS:41:VAL:HG13 | 19:QS:44:MET:HB2   | 1.57                     | 0.87              |
| 20:QT:23:ARG:HA   | 20:QT:26:ASN:HD21  | 1.37                     | 0.87              |
| 27:RD:28:GLU:HB2  | 27:RD:29:PRO:HD2   | 1.56                     | 0.87              |
| 19:XS:8:GLY:O     | 19:XS:9:VAL:HG22   | 1.74                     | 0.87              |
| 25:YA:637:A:H2'   | 35:YP:117:GLU:OE2  | 1.74                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Y1:82:LEU:HD13  | 47:Y1:83:GLU:O     | 1.74                     | 0.87              |
| 2:QB:96:ARG:H      | 2:QB:96:ARG:HD2    | 1.38                     | 0.87              |
| 14:QN:12:ARG:C     | 14:QN:14:PRO:HD2   | 1.98                     | 0.87              |
| 47:Y1:82:LEU:HD11  | 47:Y1:83:GLU:O     | 1.75                     | 0.87              |
| 27:RD:181:GLU:HA   | 27:RD:272:ALA:HB3  | 1.57                     | 0.87              |
| 27:YD:181:GLU:HA   | 27:YD:272:ALA:HB3  | 1.57                     | 0.87              |
| 36:YQ:64:ILE:HA    | 36:YQ:106:VAL:HG12 | 1.54                     | 0.87              |
| 21:QU:6:ARG:HE     | 21:QU:15:ARG:CZ    | 1.87                     | 0.87              |
| 25:RA:247:G:O6     | 54:R8:12:LYS:NZ    | 2.06                     | 0.87              |
| 35:RP:64:LYS:O     | 35:RP:66:GLY:N     | 2.07                     | 0.87              |
| 11:XK:32:ILE:HD12  | 11:XK:72:ALA:HB2   | 1.56                     | 0.87              |
| 22:XV:75:C:OP1     | 25:YA:2602:A:OP1   | 1.92                     | 0.87              |
| 15:QO:56:LEU:O     | 15:QO:60:VAL:HG23  | 1.75                     | 0.87              |
| 27:RD:44:ASN:HD22  | 27:RD:44:ASN:H     | 1.19                     | 0.87              |
| 10:XJ:74:ILE:H     | 10:XJ:74:ILE:HD13  | 1.38                     | 0.87              |
| 10:QJ:47:PHE:HE1   | 10:QJ:63:PHE:HB2   | 1.40                     | 0.87              |
| 24:QX:2:U:O2'      | 24:QX:3:G:H5'      | 1.73                     | 0.87              |
| 36:RQ:64:ILE:HA    | 36:RQ:106:VAL:HG12 | 1.54                     | 0.87              |
| 8:XH:51:VAL:HG21   | 8:XH:60:ARG:HG2    | 1.55                     | 0.87              |
| 13:XM:4:ILE:H      | 13:XM:9:ILE:CG2    | 1.88                     | 0.87              |
| 19:QS:8:GLY:O      | 19:QS:9:VAL:HG22   | 1.75                     | 0.86              |
| 38:RS:106:ARG:HB2  | 38:RS:106:ARG:HH11 | 1.39                     | 0.86              |
| 47:R1:92:LYS:HG3   | 47:R1:96:LYS:HB2   | 1.57                     | 0.86              |
| 10:XJ:7:LYS:HB2    | 10:XJ:97:GLU:HB2   | 1.56                     | 0.86              |
| 13:XM:97:PRO:HB2   | 13:XM:101:GLN:NE2  | 1.89                     | 0.86              |
| 30:YG:145:THR:HG23 | 50:Y4:28:LYS:HZ1   | 1.38                     | 0.86              |
| 30:RG:116:ASP:O    | 30:RG:117:PHE:HB3  | 1.72                     | 0.86              |
| 30:YG:101:ILE:HG13 | 30:YG:102:PHE:N    | 1.86                     | 0.86              |
| 35:YP:18:ARG:O     | 35:YP:19:VAL:HB    | 1.75                     | 0.86              |
| 19:QS:27:GLU:O     | 19:QS:28:LYS:HG2   | 1.74                     | 0.86              |
| 35:RP:75:ILE:HD13  | 35:RP:75:ILE:H     | 1.39                     | 0.86              |
| 29:RF:82:ILE:O     | 29:RF:82:ILE:HG13  | 1.73                     | 0.86              |
| 19:XS:27:GLU:O     | 19:XS:28:LYS:HG2   | 1.74                     | 0.86              |
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H    | 1.39                     | 0.86              |
| 40:YU:92:ARG:HD2   | 41:YV:11:GLN:NE2   | 1.90                     | 0.86              |
| 29:YF:7:TYR:HB3    | 29:YF:21:ALA:HB1   | 1.53                     | 0.86              |
| 5:QE:71:LEU:O      | 5:QE:72:GLN:HG3    | 1.73                     | 0.86              |
| 1:XA:954:G:H4'     | 13:XM:121:LYS:HG3  | 1.55                     | 0.86              |
| 27:YD:35:LYS:HG2   | 27:YD:64:ILE:H     | 1.40                     | 0.86              |
| 2:QB:67:THR:HG21   | 2:QB:155:LEU:HD21  | 1.57                     | 0.86              |
| 11:QK:32:ILE:HD12  | 11:QK:72:ALA:HB2   | 1.56                     | 0.86              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:44:ASN:CB    | 27:RD:49:ILE:HA    | 2.04                     | 0.86              |
| 30:RG:161:THR:HG22 | 30:RG:163:ALA:H    | 1.39                     | 0.86              |
| 2:XB:96:ARG:H      | 2:XB:96:ARG:HD2    | 1.38                     | 0.86              |
| 31:YH:127:GLU:HG2  | 31:YH:128:PRO:HD3  | 0.86                     | 0.86              |
| 4:QD:114:ARG:HH11  | 4:QD:114:ARG:HG3   | 1.39                     | 0.86              |
| 25:RA:571:A:O2'    | 41:RV:78:LYS:NZ    | 2.09                     | 0.86              |
| 38:YS:106:ARG:HB2  | 38:YS:106:ARG:HH11 | 1.39                     | 0.86              |
| 41:YV:19:LYS:HD2   | 41:YV:95:LEU:HD23  | 1.55                     | 0.86              |
| 13:QM:14:ARG:H     | 13:QM:44:ARG:HD3   | 1.41                     | 0.86              |
| 31:RH:8:PRO:C      | 31:RH:9:ILE:HG12   | 2.00                     | 0.86              |
| 44:RY:51:VAL:O     | 44:RY:56:PRO:HA    | 1.76                     | 0.86              |
| 2:XB:67:THR:HG21   | 2:XB:155:LEU:HD21  | 1.56                     | 0.86              |
| 19:XS:41:VAL:HG13  | 19:XS:44:MET:HB2   | 1.56                     | 0.86              |
| 13:QM:4:ILE:H      | 13:QM:9:ILE:CG2    | 1.88                     | 0.86              |
| 10:QJ:49:VAL:HG13  | 14:QN:41:ARG:HD2   | 0.94                     | 0.85              |
| 28:RE:61:ARG:O     | 28:RE:63:LEU:HG    | 1.77                     | 0.85              |
| 2:QB:178:ARG:HH21  | 8:QH:74:PRO:HB3    | 1.39                     | 0.85              |
| 4:QD:22:LYS:CB     | 4:QD:26:CYS:SG     | 2.64                     | 0.85              |
| 40:RU:92:ARG:HD2   | 41:RV:11:GLN:NE2   | 1.90                     | 0.85              |
| 10:XJ:53:PRO:O     | 14:YN:41:ARG:NH2   | 2.09                     | 0.85              |
| 25:RA:1826:G:H4'   | 27:RD:242:ARG:HH21 | 1.41                     | 0.85              |
| 47:R1:82:LEU:HD13  | 47:R1:83:GLU:O     | 1.74                     | 0.85              |
| 36:YQ:75:THR:HA    | 36:YQ:88:GLY:O     | 1.75                     | 0.85              |
| 5:QE:78:HIS:CD2    | 8:QH:104:ARG:HG2   | 2.11                     | 0.85              |
| 29:RF:32:LEU:HD13  | 29:RF:105:VAL:HG13 | 1.59                     | 0.85              |
| 4:QD:166:LYS:HG2   | 27:YD:134:ARG:NH1  | 1.92                     | 0.85              |
| 36:RQ:75:THR:HA    | 36:RQ:88:GLY:O     | 1.76                     | 0.85              |
| 35:YP:101:VAL:HG23 | 35:YP:107:LYS:H    | 1.41                     | 0.85              |
| 20:QT:36:LEU:HD13  | 20:QT:39:LYS:HD3   | 1.57                     | 0.85              |
| 28:RE:95:ILE:H     | 28:RE:95:ILE:HD12  | 1.41                     | 0.85              |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:HZ1   | 1.39                     | 0.85              |
| 15:XO:56:LEU:O     | 15:XO:60:VAL:HG23  | 1.75                     | 0.85              |
| 31:YH:89:ILE:HD11  | 31:YH:129:THR:HB   | 1.58                     | 0.85              |
| 35:YP:75:ILE:H     | 35:YP:75:ILE:HD13  | 1.39                     | 0.85              |
| 39:YT:111:ARG:O    | 39:YT:112:ARG:HG3  | 1.76                     | 0.85              |
| 28:RE:81:ILE:O     | 28:RE:82:ARG:HB2   | 1.75                     | 0.85              |
| 51:R5:39:MET:O     | 51:R5:40:LYS:HG3   | 1.77                     | 0.85              |
| 44:YY:51:VAL:O     | 44:YY:56:PRO:HA    | 1.76                     | 0.85              |
| 31:RH:127:GLU:HG2  | 31:RH:128:PRO:HD3  | 0.86                     | 0.85              |
| 40:RU:64:ARG:HG2   | 40:RU:64:ARG:HH21  | 1.42                     | 0.85              |
| 5:XE:51:VAL:HB     | 5:XE:52:PRO:HD3    | 1.59                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:XO:3:ILE:HD13  | 15:XO:3:ILE:H      | 1.40                     | 0.85              |
| 20:XT:36:LEU:HD13 | 20:XT:39:LYS:HD3   | 1.57                     | 0.85              |
| 26:YB:44:G:OP1    | 50:Y4:1:MET:N      | 2.08                     | 0.85              |
| 30:YG:67:LYS:HE2  | 50:Y4:6:HIS:NE2    | 1.92                     | 0.85              |
| 54:Y8:59:LYS:NZ   | 54:Y8:59:LYS:CB    | 2.39                     | 0.85              |
| 27:RD:17:THR:HG22 | 27:RD:205:VAL:H    | 1.41                     | 0.85              |
| 30:RG:67:LYS:HE2  | 50:R4:6:HIS:NE2    | 1.92                     | 0.85              |
| 7:XG:44:TYR:HA    | 7:XG:47:CYS:SG     | 2.17                     | 0.85              |
| 27:YD:28:GLU:HB2  | 27:YD:29:PRO:HD2   | 1.56                     | 0.85              |
| 29:YF:82:ILE:O    | 29:YF:82:ILE:HG13  | 1.73                     | 0.85              |
| 1:QA:1123:A:H4'   | 10:QJ:36:GLY:HA3   | 1.59                     | 0.84              |
| 10:QJ:49:VAL:HG21 | 14:QN:41:ARG:HB2   | 1.23                     | 0.84              |
| 25:RA:819:A:OP2   | 25:RA:1187:G:N2    | 2.09                     | 0.84              |
| 35:RP:18:ARG:O    | 35:RP:19:VAL:HB    | 1.75                     | 0.84              |
| 54:R8:59:LYS:NZ   | 54:R8:59:LYS:CB    | 2.40                     | 0.84              |
| 2:XB:212:GLN:CD   | 2:XB:235:SER:HB2   | 2.02                     | 0.84              |
| 28:YE:95:ILE:HD12 | 28:YE:95:ILE:H     | 1.42                     | 0.84              |
| 38:YS:106:ARG:HA  | 38:YS:110:LEU:CD1  | 2.07                     | 0.84              |
| 13:XM:14:ARG:H    | 13:XM:44:ARG:HD3   | 1.41                     | 0.84              |
| 31:YH:8:PRO:C     | 31:YH:9:ILE:HG12   | 2.00                     | 0.84              |
| 10:QJ:49:VAL:CB   | 14:QN:41:ARG:HB2   | 2.08                     | 0.84              |
| 14:QN:23:ARG:O    | 14:QN:24:CYS:O     | 1.95                     | 0.84              |
| 31:RH:89:ILE:HD11 | 31:RH:129:THR:HB   | 1.59                     | 0.84              |
| 38:YS:83:LYS:HG2  | 38:YS:109:GLY:CA   | 2.07                     | 0.84              |
| 41:YV:49:THR:HB   | 41:YV:50:PRO:CD    | 2.07                     | 0.84              |
| 10:QJ:7:LYS:HB2   | 10:QJ:97:GLU:HB2   | 1.57                     | 0.84              |
| 15:QO:82:ILE:HD11 | 15:QO:88:ARG:CG    | 2.07                     | 0.84              |
| 25:RA:2056:G:N2   | 51:R5:4:HIS:O      | 2.09                     | 0.84              |
| 13:XM:23:TYR:HB3  | 13:XM:67:GLU:HG2   | 1.59                     | 0.84              |
| 27:YD:17:THR:HG22 | 27:YD:205:VAL:H    | 1.41                     | 0.84              |
| 28:YE:81:ILE:O    | 28:YE:82:ARG:HB2   | 1.75                     | 0.84              |
| 30:YG:98:ARG:HA   | 30:YG:101:ILE:HG12 | 1.59                     | 0.84              |
| 7:QG:44:TYR:HA    | 7:QG:47:CYS:SG     | 2.17                     | 0.84              |
| 14:QN:21:TYR:HE2  | 14:QN:23:ARG:HH21  | 1.24                     | 0.84              |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:HG11 | 1.59                     | 0.84              |
| 28:YE:61:ARG:O    | 28:YE:63:LEU:HG    | 1.77                     | 0.84              |
| 34:YO:26:LYS:HB2  | 34:YO:30:ALA:HB2   | 1.59                     | 0.84              |
| 35:RP:62:LEU:CD2  | 54:R8:25:MET:HB2   | 2.08                     | 0.84              |
| 38:RS:89:ARG:HD2  | 38:RS:92:TYR:O     | 1.78                     | 0.84              |
| 1:XA:1139:G:N2    | 1:XA:1143:G:O6     | 2.09                     | 0.84              |
| 25:YA:2068:U:H3   | 25:YA:2430:A:H2    | 1.25                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:54:ARG:NH1   | 31:YH:62:LYS:HG2   | 1.92                     | 0.84              |
| 51:Y5:40:LYS:HD3   | 51:Y5:46:CYS:HB3   | 1.60                     | 0.84              |
| 30:RG:98:ARG:HA    | 30:RG:101:ILE:HG12 | 1.59                     | 0.84              |
| 34:RO:26:LYS:HB2   | 34:RO:30:ALA:HB2   | 1.59                     | 0.84              |
| 10:XJ:4:ILE:HB     | 10:XJ:74:ILE:HD11  | 1.60                     | 0.84              |
| 35:YP:62:LEU:CD2   | 54:Y8:25:MET:HB2   | 2.08                     | 0.84              |
| 36:YQ:30:GLY:HA2   | 36:YQ:107:ALA:HB2  | 1.60                     | 0.84              |
| 44:YY:57:GLN:NE2   | 44:YY:58:GLY:H     | 1.76                     | 0.84              |
| 2:QB:212:GLN:CD    | 2:QB:235:SER:HB2   | 2.02                     | 0.84              |
| 17:QQ:59:ILE:HG22  | 17:QQ:73:VAL:HA    | 1.60                     | 0.84              |
| 25:RA:674:G:H1'    | 29:RF:74:ARG:HD3   | 1.58                     | 0.84              |
| 38:RS:83:LYS:HG2   | 38:RS:109:GLY:CA   | 2.07                     | 0.84              |
| 39:RT:111:ARG:O    | 39:RT:112:ARG:HG3  | 1.76                     | 0.84              |
| 41:RV:49:THR:HB    | 41:RV:50:PRO:CD    | 2.07                     | 0.84              |
| 10:XJ:37:PRO:HA    | 10:XJ:72:VAL:HG22  | 1.59                     | 0.84              |
| 14:YN:32:SER:OG    | 14:YN:41:ARG:CB    | 2.25                     | 0.84              |
| 29:YF:53:THR:HG23  | 29:YF:56:GLU:OE1   | 1.77                     | 0.84              |
| 31:RH:54:ARG:NH1   | 31:RH:62:LYS:HG2   | 1.92                     | 0.84              |
| 38:YS:89:ARG:HD2   | 38:YS:92:TYR:O     | 1.78                     | 0.84              |
| 14:QN:8:GLU:OE2    | 14:QN:11:LYS:HD2   | 1.78                     | 0.84              |
| 27:RD:35:LYS:HG2   | 27:RD:64:ILE:H     | 1.40                     | 0.84              |
| 8:XH:1:MET:HE2     | 8:XH:1:MET:H3      | 1.43                     | 0.84              |
| 25:YA:2056:G:N2    | 51:Y5:4:HIS:O      | 2.09                     | 0.84              |
| 39:YT:3:ARG:HG3    | 39:YT:7:ILE:HG12   | 1.60                     | 0.84              |
| 4:QD:22:LYS:HB2    | 4:QD:26:CYS:SG     | 2.18                     | 0.83              |
| 47:R1:82:LEU:HD11  | 47:R1:83:GLU:O     | 1.75                     | 0.83              |
| 15:XO:82:ILE:HD11  | 15:XO:88:ARG:CG    | 2.07                     | 0.83              |
| 4:QD:96:LEU:HD22   | 4:QD:96:LEU:H      | 1.43                     | 0.83              |
| 5:QE:81:GLU:HB3    | 5:QE:90:VAL:HG22   | 1.60                     | 0.83              |
| 39:RT:24:PRO:HA    | 39:RT:49:VAL:HG13  | 1.59                     | 0.83              |
| 44:RY:81:LYS:HD3   | 44:RY:97:ARG:HE    | 1.43                     | 0.83              |
| 25:YA:2404:C:H1'   | 35:YP:67:MET:HE1   | 1.60                     | 0.83              |
| 37:YR:117:VAL:HG22 | 37:YR:118:GLU:H    | 1.43                     | 0.83              |
| 47:Y1:92:LYS:HG3   | 47:Y1:96:LYS:HB2   | 1.58                     | 0.83              |
| 52:Y6:27:LYS:HB2   | 52:Y6:27:LYS:NZ    | 1.93                     | 0.83              |
| 4:QD:25:ARG:NH1    | 4:QD:30:LYS:HE3    | 1.93                     | 0.83              |
| 5:QE:51:VAL:HB     | 5:QE:52:PRO:HD3    | 1.59                     | 0.83              |
| 25:RA:338:G:OP1    | 44:RY:4:LYS:NZ     | 2.10                     | 0.83              |
| 31:RH:105:LEU:HD13 | 31:RH:105:LEU:H    | 1.42                     | 0.83              |
| 51:R5:40:LYS:HD3   | 51:R5:46:CYS:HB3   | 1.60                     | 0.83              |
| 3:XC:15:THR:CG2    | 3:XC:181:ASN:HA    | 2.08                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:47:PHE:HE1   | 10:XJ:63:PHE:HB2   | 1.40                     | 0.83              |
| 35:YP:126:VAL:HG22 | 35:YP:145:PRO:HG2  | 1.61                     | 0.83              |
| 13:QM:23:TYR:HB3   | 13:QM:67:GLU:HG2   | 1.60                     | 0.83              |
| 37:RR:117:VAL:HG22 | 37:RR:118:GLU:H    | 1.43                     | 0.83              |
| 14:XN:8:GLU:OE2    | 14:XN:11:LYS:HD2   | 1.78                     | 0.83              |
| 29:YF:32:LEU:HD13  | 29:YF:105:VAL:HG13 | 1.59                     | 0.83              |
| 31:YH:13:LYS:HE2   | 31:YH:13:LYS:HA    | 1.61                     | 0.83              |
| 51:Y5:39:MET:O     | 51:Y5:40:LYS:HG3   | 1.77                     | 0.83              |
| 10:QJ:37:PRO:HA    | 10:QJ:72:VAL:HG22  | 1.59                     | 0.83              |
| 28:RE:35:GLN:HG2   | 28:RE:37:ARG:HE    | 1.44                     | 0.83              |
| 33:RN:133:GLN:HB2  | 33:RN:135:PRO:HD3  | 1.59                     | 0.83              |
| 44:RY:57:GLN:NE2   | 44:RY:58:GLY:H     | 1.76                     | 0.83              |
| 25:YA:2451:A:C6    | 56:Z8:76:PPU:HE2   | 2.14                     | 0.83              |
| 33:YN:131:GLN:NE2  | 33:YN:132:ALA:H    | 1.75                     | 0.83              |
| 39:RT:3:ARG:HG3    | 39:RT:7:ILE:HG12   | 1.60                     | 0.83              |
| 35:YP:59:LEU:HA    | 35:YP:61:ARG:HH21  | 1.44                     | 0.83              |
| 45:YZ:151:HIS:HB3  | 45:YZ:170:THR:HA   | 1.61                     | 0.83              |
| 1:QA:346:G:OP1     | 39:RT:41:ARG:NH2   | 2.12                     | 0.83              |
| 19:QS:50:ALA:HB1   | 19:QS:57:HIS:HB3   | 1.60                     | 0.83              |
| 29:RF:192:LEU:HD21 | 29:RF:194:MET:HE3  | 1.59                     | 0.83              |
| 35:RP:65:ARG:HG3   | 35:RP:65:ARG:NH1   | 1.90                     | 0.83              |
| 1:XA:1106:G:H5"    | 3:XC:172:ARG:HG2   | 1.60                     | 0.83              |
| 7:XG:78:ARG:HG3    | 7:XG:79:ARG:N      | 1.93                     | 0.83              |
| 33:RN:131:GLN:NE2  | 33:RN:132:ALA:H    | 1.75                     | 0.83              |
| 35:RP:138:LEU:C    | 35:RP:140:ALA:H    | 1.85                     | 0.83              |
| 39:RT:53:ARG:O     | 39:RT:59:THR:HG23  | 1.78                     | 0.83              |
| 41:RV:66:ARG:NH1   | 41:RV:88:ARG:HD3   | 1.94                     | 0.83              |
| 50:R4:36:CYS:O     | 50:R4:39:CYS:HB2   | 1.79                     | 0.83              |
| 28:YE:7:VAL:HG23   | 28:YE:8:LYS:H      | 1.44                     | 0.83              |
| 39:YT:53:ARG:O     | 39:YT:59:THR:HG23  | 1.78                     | 0.83              |
| 15:QO:3:ILE:H      | 15:QO:3:ILE:HD13   | 1.40                     | 0.83              |
| 29:RF:53:THR:HG23  | 29:RF:56:GLU:OE1   | 1.77                     | 0.83              |
| 38:RS:88:ASP:O     | 38:RS:89:ARG:HB3   | 1.78                     | 0.83              |
| 2:QB:193:ASP:OD2   | 2:QB:196:LEU:HG    | 1.78                     | 0.82              |
| 7:QG:78:ARG:HG3    | 7:QG:79:ARG:N      | 1.93                     | 0.82              |
| 12:QL:38:THR:HG23  | 12:QL:39:VAL:HG23  | 1.60                     | 0.82              |
| 35:RP:101:VAL:HG23 | 35:RP:107:LYS:H    | 1.41                     | 0.82              |
| 2:XB:204:ASN:ND2   | 2:XB:206:ASP:H     | 1.77                     | 0.82              |
| 33:YN:133:GLN:HB2  | 33:YN:135:PRO:HD3  | 1.59                     | 0.82              |
| 2:QB:204:ASN:ND2   | 2:QB:206:ASP:H     | 1.77                     | 0.82              |
| 4:QD:166:LYS:CG    | 27:YD:134:ARG:NH1  | 2.41                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:166:LYS:HD2   | 27:YD:134:ARG:HH12 | 1.44                     | 0.82              |
| 28:RE:15:PHE:CE1   | 28:RE:20:ALA:HB2   | 2.14                     | 0.82              |
| 36:RQ:30:GLY:HA2   | 36:RQ:107:ALA:HB2  | 1.60                     | 0.82              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:CD1  | 2.08                     | 0.82              |
| 2:XB:185:ILE:HG22  | 2:XB:199:TYR:HB2   | 1.60                     | 0.82              |
| 14:YN:44:LEU:HD12  | 14:YN:53:LEU:CD1   | 2.08                     | 0.82              |
| 31:YH:105:LEU:HD13 | 31:YH:105:LEU:H    | 1.42                     | 0.82              |
| 3:QC:113:ALA:HB3   | 3:QC:114:PRO:HD3   | 1.62                     | 0.82              |
| 25:RA:2314:C:OP1   | 30:RG:91:ARG:NH1   | 2.10                     | 0.82              |
| 52:R6:27:LYS:HB2   | 52:R6:27:LYS:NZ    | 1.93                     | 0.82              |
| 19:XS:50:ALA:HB1   | 19:XS:57:HIS:HB3   | 1.60                     | 0.82              |
| 27:YD:25:THR:CG2   | 27:YD:82:ILE:H     | 1.93                     | 0.82              |
| 27:YD:35:LYS:HZ1   | 27:YD:104:TYR:HB2  | 1.44                     | 0.82              |
| 28:YE:15:PHE:CE1   | 28:YE:20:ALA:HB2   | 2.14                     | 0.82              |
| 39:YT:24:PRO:HA    | 39:YT:49:VAL:HG13  | 1.59                     | 0.82              |
| 10:QJ:49:VAL:HG11  | 14:QN:41:ARG:HB2   | 1.58                     | 0.82              |
| 4:XD:96:LEU:H      | 4:XD:96:LEU:HD22   | 1.43                     | 0.82              |
| 5:XE:81:GLU:HB3    | 5:XE:90:VAL:HG22   | 1.59                     | 0.82              |
| 11:XK:124:LYS:HD2  | 11:XK:125:PHE:HE1  | 1.45                     | 0.82              |
| 31:YH:153:LYS:HG2  | 31:YH:162:ILE:HG13 | 1.61                     | 0.82              |
| 40:YU:64:ARG:HG2   | 40:YU:64:ARG:HH21  | 1.42                     | 0.82              |
| 25:RA:2502:G:H5''  | 25:RA:2503:A:H5''  | 1.62                     | 0.82              |
| 27:RD:35:LYS:NZ    | 27:RD:104:TYR:HB2  | 1.93                     | 0.82              |
| 30:RG:127:GLY:HA2  | 30:RG:166:ASP:CG   | 2.05                     | 0.82              |
| 52:R6:15:GLU:CD    | 52:R6:41:PRO:HB3   | 2.04                     | 0.82              |
| 2:XB:193:ASP:OD2   | 2:XB:196:LEU:HG    | 1.79                     | 0.82              |
| 12:XL:38:THR:HG23  | 12:XL:39:VAL:HG23  | 1.60                     | 0.82              |
| 44:YY:81:LYS:HD3   | 44:YY:97:ARG:HE    | 1.43                     | 0.82              |
| 2:QB:185:ILE:HG22  | 2:QB:199:TYR:HB2   | 1.61                     | 0.82              |
| 14:QN:41:ARG:NH2   | 14:QN:42:ILE:HD11  | 1.94                     | 0.82              |
| 28:RE:7:VAL:HG23   | 28:RE:8:LYS:H      | 1.44                     | 0.82              |
| 16:XP:4:ILE:CD1    | 16:XP:64:ALA:HB1   | 2.08                     | 0.82              |
| 17:XQ:59:ILE:HG22  | 17:XQ:73:VAL:HA    | 1.60                     | 0.82              |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:HE3  | 1.59                     | 0.82              |
| 40:YU:88:ILE:HD13  | 40:YU:88:ILE:H     | 1.44                     | 0.82              |
| 40:RU:88:ILE:HD13  | 40:RU:88:ILE:H     | 1.44                     | 0.82              |
| 50:R4:33:VAL:HG12  | 50:R4:34:GLU:H     | 1.44                     | 0.82              |
| 2:XB:84:GLU:OE1    | 2:XB:216:SER:HA    | 1.80                     | 0.82              |
| 27:YD:35:LYS:NZ    | 27:YD:104:TYR:HB2  | 1.93                     | 0.82              |
| 30:YG:127:GLY:HA2  | 30:YG:166:ASP:CG   | 2.05                     | 0.82              |
| 33:YN:22:THR:HG22  | 33:YN:23:LEU:H     | 1.44                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:YO:14:THR:HG21  | 34:YO:86:ILE:HB    | 1.62                     | 0.82              |
| 50:Y4:36:CYS:O     | 50:Y4:39:CYS:HB2   | 1.80                     | 0.82              |
| 2:QB:21:ARG:HG3    | 2:QB:38:GLY:C      | 2.05                     | 0.82              |
| 38:YS:19:LYS:O     | 38:YS:20:ARG:HB3   | 1.80                     | 0.82              |
| 48:Y2:16:LEU:O     | 48:Y2:16:LEU:HG    | 1.78                     | 0.82              |
| 30:RG:179:PRO:HG3  | 50:R4:38:LYS:NZ    | 1.95                     | 0.82              |
| 33:RN:22:THR:HG22  | 33:RN:23:LEU:H     | 1.44                     | 0.82              |
| 30:YG:179:PRO:HG3  | 50:Y4:38:LYS:NZ    | 1.95                     | 0.82              |
| 39:YT:102:ILE:HA   | 39:YT:105:LEU:HD21 | 1.62                     | 0.82              |
| 50:Y4:71:ARG:HG3   | 50:Y4:71:ARG:NH1   | 1.90                     | 0.82              |
| 25:RA:2068:U:H3    | 25:RA:2430:A:H2    | 1.24                     | 0.81              |
| 35:YP:39:LYS:HA    | 35:YP:45:LEU:CD1   | 2.10                     | 0.81              |
| 2:QB:84:GLU:OE1    | 2:QB:216:SER:HA    | 1.80                     | 0.81              |
| 2:QB:196:LEU:CD1   | 2:QB:197:VAL:HG23  | 2.10                     | 0.81              |
| 12:QL:86:ARG:HB2   | 12:QL:101:VAL:HG22 | 1.62                     | 0.81              |
| 29:RF:155:LEU:HD13 | 29:RF:174:VAL:HG13 | 1.62                     | 0.81              |
| 31:RH:132:ARG:HB2  | 31:RH:132:ARG:NH1  | 1.94                     | 0.81              |
| 25:YA:2308:G:H22   | 25:YA:2311:A:H2    | 1.28                     | 0.81              |
| 52:Y6:15:GLU:CD    | 52:Y6:41:PRO:HB3   | 2.04                     | 0.81              |
| 10:QJ:63:PHE:HD1   | 14:QN:58:LYS:HA    | 1.44                     | 0.81              |
| 16:QP:4:ILE:CD1    | 16:QP:64:ALA:HB1   | 2.09                     | 0.81              |
| 16:QP:51:VAL:HG12  | 16:QP:52:ASP:H     | 1.46                     | 0.81              |
| 31:RH:152:ARG:O    | 31:RH:153:LYS:HB2  | 1.80                     | 0.81              |
| 31:RH:153:LYS:HG2  | 31:RH:162:ILE:HG13 | 1.61                     | 0.81              |
| 35:RP:126:VAL:HG22 | 35:RP:145:PRO:HG2  | 1.60                     | 0.81              |
| 36:RQ:83:MET:HB2   | 46:R0:7:LEU:HD12   | 1.59                     | 0.81              |
| 36:RQ:90:VAL:HG13  | 36:RQ:91:GLU:N     | 1.95                     | 0.81              |
| 48:R2:16:LEU:O     | 48:R2:16:LEU:HG    | 1.78                     | 0.81              |
| 54:R8:52:LYS:N     | 54:R8:53:PRO:CD    | 2.43                     | 0.81              |
| 2:XB:122:PHE:HD1   | 2:XB:139:LYS:HZ1   | 1.27                     | 0.81              |
| 10:XJ:6:ILE:O      | 10:XJ:6:ILE:HD12   | 1.81                     | 0.81              |
| 30:YG:67:LYS:HE2   | 50:Y4:6:HIS:CE1    | 2.14                     | 0.81              |
| 31:YH:10:PRO:O     | 31:YH:11:VAL:HG13  | 1.80                     | 0.81              |
| 36:YQ:90:VAL:HG13  | 36:YQ:91:GLU:N     | 1.95                     | 0.81              |
| 38:YS:88:ASP:O     | 38:YS:89:ARG:HB3   | 1.78                     | 0.81              |
| 41:YV:66:ARG:NH1   | 41:YV:88:ARG:HD3   | 1.94                     | 0.81              |
| 53:Y7:48:LYS:HG2   | 53:Y7:49:ARG:H     | 1.45                     | 0.81              |
| 34:RO:53:LYS:HD2   | 34:RO:53:LYS:N     | 1.96                     | 0.81              |
| 3:XC:113:ALA:HB3   | 3:XC:114:PRO:HD3   | 1.61                     | 0.81              |
| 4:XD:108:LEU:HD11  | 4:XD:174:LEU:HD22  | 1.60                     | 0.81              |
| 10:XJ:63:PHE:HD1   | 14:YN:58:LYS:HA    | 1.43                     | 0.81              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 28:YE:24:THR:HG21   | 28:YE:188:VAL:HG11 | 1.59                     | 0.81              |
| 30:YG:47:LYS:HD3    | 30:YG:81:LYS:HB2   | 1.63                     | 0.81              |
| 4:QD:166:LYS:CD     | 27:YD:134:ARG:HH12 | 1.91                     | 0.81              |
| 10:QJ:4:ILE:HB      | 10:QJ:74:ILE:HD11  | 1.60                     | 0.81              |
| 39:RT:102:ILE:HA    | 39:RT:105:LEU:HD21 | 1.62                     | 0.81              |
| 3:QC:15:THR:CG2     | 3:QC:181:ASN:HA    | 2.08                     | 0.81              |
| 4:QD:108:LEU:HD11   | 4:QD:174:LEU:HD22  | 1.60                     | 0.81              |
| 25:RA:141:A:H8      | 25:RA:1595:G:H21   | 1.27                     | 0.81              |
| 25:RA:631:A:OP2     | 54:R8:46:ARG:NH2   | 2.13                     | 0.81              |
| 27:RD:27:THR:HG23   | 27:RD:28:GLU:N     | 1.96                     | 0.81              |
| 30:RG:67:LYS:HE2    | 50:R4:6:HIS:CE1    | 2.14                     | 0.81              |
| 33:RN:35:ARG:HG3    | 33:RN:37:LYS:HG3   | 1.63                     | 0.81              |
| 5:XE:78:HIS:CD2     | 8:XH:104:ARG:HG2   | 2.16                     | 0.81              |
| 1:QA:973:G:OP1      | 10:QJ:57:LYS:NZ    | 2.13                     | 0.81              |
| 1:QA:1151:A:H1'     | 10:QJ:39:PRO:HB2   | 1.62                     | 0.81              |
| 7:QG:111:ARG:HH11   | 7:QG:111:ARG:HB3   | 1.46                     | 0.81              |
| 28:RE:3:GLY:O       | 28:RE:4:ILE:HB     | 1.81                     | 0.81              |
| 35:RP:39:LYS:HA     | 35:RP:45:LEU:CD1   | 2.10                     | 0.81              |
| 48:R2:43:GLN:O      | 48:R2:44:LEU:HG    | 1.81                     | 0.81              |
| 53:R7:48:LYS:HG2    | 53:R7:49:ARG:H     | 1.46                     | 0.81              |
| 25:YA:1142(A):A:H4' | 33:YN:25:ARG:HH22  | 1.46                     | 0.81              |
| 28:YE:116:VAL:HG21  | 28:YE:122:PHE:CD2  | 2.16                     | 0.81              |
| 38:RS:36:TYR:HD2    | 38:RS:52:SER:HB3   | 1.46                     | 0.81              |
| 38:RS:106:ARG:CA    | 38:RS:110:LEU:HD21 | 2.11                     | 0.81              |
| 1:XA:973:G:OP1      | 10:XJ:57:LYS:NZ    | 2.12                     | 0.81              |
| 35:YP:138:LEU:C     | 35:YP:140:ALA:H    | 1.85                     | 0.81              |
| 13:QM:77:ASN:HA     | 50:R4:71:ARG:NH2   | 1.96                     | 0.81              |
| 39:RT:39:ARG:HG2    | 39:RT:40:THR:H     | 1.46                     | 0.81              |
| 4:XD:30:LYS:C       | 4:XD:32:ALA:N      | 2.36                     | 0.81              |
| 28:YE:50:GLY:CA     | 28:YE:77:ILE:HA    | 2.10                     | 0.81              |
| 29:YF:155:LEU:HD13  | 29:YF:174:VAL:HG13 | 1.62                     | 0.81              |
| 33:YN:35:ARG:HG3    | 33:YN:37:LYS:HG3   | 1.63                     | 0.81              |
| 48:Y2:43:GLN:O      | 48:Y2:44:LEU:HG    | 1.81                     | 0.81              |
| 3:QC:47:LEU:HD11    | 3:QC:76:VAL:HG12   | 1.62                     | 0.81              |
| 10:QJ:6:ILE:HD12    | 10:QJ:6:ILE:O      | 1.81                     | 0.81              |
| 39:RT:62:THR:CG2    | 39:RT:75:ILE:HG12  | 2.11                     | 0.81              |
| 33:YN:43:THR:HB     | 33:YN:46:VAL:HG12  | 1.63                     | 0.81              |
| 3:QC:52:LEU:H       | 3:QC:52:LEU:HD23   | 1.46                     | 0.80              |
| 25:RA:957:A:H5'     | 36:RQ:76:LYS:HD2   | 1.62                     | 0.80              |
| 25:RA:1138:G:H21    | 33:RN:106:MET:HE3  | 1.45                     | 0.80              |
| 25:RA:2245:U:H5'    | 25:RA:2246:G:H5'   | 1.63                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:47:LYS:HD3   | 30:RG:81:LYS:HB2   | 1.63                     | 0.80              |
| 44:RY:76:CYS:HB3   | 44:RY:96:ILE:CD1   | 2.07                     | 0.80              |
| 3:XC:47:LEU:HD11   | 3:XC:76:VAL:HG12   | 1.61                     | 0.80              |
| 39:YT:39:ARG:HG2   | 39:YT:40:THR:H     | 1.46                     | 0.80              |
| 28:RE:52:LEU:HB2   | 28:RE:75:VAL:HG23  | 1.62                     | 0.80              |
| 28:RE:116:VAL:HG21 | 28:RE:122:PHE:CD2  | 2.16                     | 0.80              |
| 31:RH:13:LYS:HE2   | 31:RH:13:LYS:HA    | 1.61                     | 0.80              |
| 51:R5:4:HIS:HB3    | 51:R5:5:PRO:CD     | 2.11                     | 0.80              |
| 2:XB:21:ARG:HG3    | 2:XB:38:GLY:C      | 2.05                     | 0.80              |
| 16:XP:51:VAL:HG12  | 16:XP:52:ASP:H     | 1.46                     | 0.80              |
| 27:YD:27:THR:HG23  | 27:YD:28:GLU:N     | 1.96                     | 0.80              |
| 38:YS:36:TYR:HD2   | 38:YS:52:SER:HB3   | 1.46                     | 0.80              |
| 44:YY:6:HIS:O      | 44:YY:7:VAL:HG13   | 1.81                     | 0.80              |
| 51:Y5:20:ARG:HA    | 51:Y5:23:HIS:HD1   | 1.46                     | 0.80              |
| 5:QE:50:GLU:HB3    | 5:QE:53:LEU:HD13   | 1.61                     | 0.80              |
| 12:QL:11:VAL:HG13  | 17:QQ:29:HIS:HD2   | 1.46                     | 0.80              |
| 14:QN:43:CYS:O     | 14:QN:44:LEU:C     | 2.22                     | 0.80              |
| 44:RY:6:HIS:O      | 44:RY:7:VAL:HG13   | 1.82                     | 0.80              |
| 54:R8:59:LYS:HB2   | 54:R8:59:LYS:HZ2   | 1.45                     | 0.80              |
| 1:XA:1071:C:H5"    | 5:XE:49:PRO:HG2    | 1.64                     | 0.80              |
| 38:YS:106:ARG:CA   | 38:YS:110:LEU:HD21 | 2.10                     | 0.80              |
| 38:RS:19:LYS:O     | 38:RS:20:ARG:HB3   | 1.80                     | 0.80              |
| 5:XE:50:GLU:HB3    | 5:XE:53:LEU:HD13   | 1.61                     | 0.80              |
| 44:YY:76:CYS:HB3   | 44:YY:96:ILE:CD1   | 2.07                     | 0.80              |
| 28:RE:50:GLY:CA    | 28:RE:77:ILE:HA    | 2.10                     | 0.80              |
| 3:XC:20:SER:HB2    | 3:XC:40:ARG:NH2    | 1.96                     | 0.80              |
| 3:XC:52:LEU:HD23   | 3:XC:52:LEU:H      | 1.46                     | 0.80              |
| 8:XH:84:ARG:HG3    | 8:XH:84:ARG:HH11   | 1.45                     | 0.80              |
| 25:YA:2580:U:H4'   | 28:YE:130:GLY:HA3  | 1.62                     | 0.80              |
| 28:YE:35:GLN:HG2   | 28:YE:37:ARG:HE    | 1.44                     | 0.80              |
| 29:YF:198:ALA:HA   | 29:YF:201:VAL:HG12 | 1.62                     | 0.80              |
| 54:Y8:52:LYS:N     | 54:Y8:53:PRO:CD    | 2.43                     | 0.80              |
| 28:RE:201:THR:CG2  | 28:RE:203:LYS:HB3  | 2.12                     | 0.80              |
| 2:XB:196:LEU:CD1   | 2:XB:197:VAL:HG23  | 2.10                     | 0.80              |
| 36:YQ:80:GLU:O     | 36:YQ:81:VAL:CG1   | 2.30                     | 0.80              |
| 50:Y4:33:VAL:HG12  | 50:Y4:34:GLU:H     | 1.44                     | 0.80              |
| 27:RD:27:THR:HG21  | 27:RD:83:GLU:HB3   | 1.64                     | 0.80              |
| 35:RP:47:ASP:OD2   | 35:RP:49:ARG:HG2   | 1.82                     | 0.80              |
| 4:XD:28:SER:HB3    | 4:XD:29:PRO:CD     | 2.12                     | 0.80              |
| 12:XL:48:PRO:HD2   | 12:XL:49:ASN:N     | 1.97                     | 0.80              |
| 28:YE:52:LEU:HB2   | 28:YE:75:VAL:HG23  | 1.62                     | 0.80              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:Y5:4:HIS:HB3   | 51:Y5:5:PRO:CD     | 2.11                     | 0.80              |
| 2:QB:4:GLU:HG2    | 2:QB:5:ILE:N       | 1.95                     | 0.80              |
| 3:QC:20:SER:HB2   | 3:QC:40:ARG:NH2    | 1.96                     | 0.80              |
| 27:RD:121:PRO:HB3 | 27:RD:135:PHE:HE1  | 1.46                     | 0.80              |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:HE1  | 1.46                     | 0.80              |
| 28:YE:3:GLY:O     | 28:YE:4:ILE:HB     | 1.81                     | 0.80              |
| 28:YE:201:THR:CG2 | 28:YE:203:LYS:HB3  | 2.12                     | 0.80              |
| 34:YO:31:LYS:HG3  | 34:YO:32:TYR:CE2   | 2.17                     | 0.80              |
| 5:QE:126:ARG:HH11 | 5:QE:126:ARG:HG3   | 1.47                     | 0.80              |
| 16:QP:4:ILE:HG13  | 16:QP:21:VAL:HG12  | 1.64                     | 0.80              |
| 27:RD:35:LYS:HZ1  | 27:RD:104:TYR:HB2  | 1.46                     | 0.80              |
| 29:RF:198:ALA:HA  | 29:RF:201:VAL:HG12 | 1.62                     | 0.80              |
| 7:XG:111:ARG:HH11 | 7:XG:111:ARG:HB3   | 1.46                     | 0.80              |
| 9:XI:19:LEU:HD23  | 9:XI:61:ALA:HB2    | 1.63                     | 0.80              |
| 14:QN:24:CYS:SG   | 14:QN:39:LEU:HA    | 2.22                     | 0.80              |
| 31:RH:150:ALA:C   | 31:RH:152:ARG:H    | 1.88                     | 0.80              |
| 41:RV:99:ILE:HD13 | 41:RV:99:ILE:N     | 1.95                     | 0.80              |
| 5:XE:126:ARG:HG3  | 5:XE:126:ARG:HH11  | 1.47                     | 0.80              |
| 30:YG:61:ALA:HB2  | 30:YG:68:PRO:CD    | 2.12                     | 0.80              |
| 4:QD:12:CYS:CA    | 4:QD:19:LEU:HD21   | 2.10                     | 0.79              |
| 8:QH:84:ARG:HH11  | 8:QH:84:ARG:HG3    | 1.44                     | 0.79              |
| 27:RD:25:THR:HG22 | 27:RD:82:ILE:H     | 1.47                     | 0.79              |
| 27:RD:34:VAL:O    | 27:RD:34:VAL:HG13  | 1.80                     | 0.79              |
| 29:RF:145:GLU:HG3 | 29:RF:145:GLU:O    | 1.81                     | 0.79              |
| 16:XP:4:ILE:HG13  | 16:XP:21:VAL:HG12  | 1.64                     | 0.79              |
| 20:XT:50:GLU:HG3  | 20:XT:51:GLU:N     | 1.97                     | 0.79              |
| 31:YH:152:ARG:O   | 31:YH:153:LYS:HB2  | 1.80                     | 0.79              |
| 41:YV:99:ILE:HD13 | 41:YV:99:ILE:N     | 1.95                     | 0.79              |
| 29:RF:11:VAL:HB   | 29:RF:18:ARG:HG3   | 1.64                     | 0.79              |
| 34:RO:14:THR:HG21 | 34:RO:86:ILE:HB    | 1.62                     | 0.79              |
| 1:XA:235:C:H5'    | 17:XQ:70:ARG:HG2   | 1.64                     | 0.79              |
| 2:XB:18:GLY:H     | 2:XB:42:ILE:CG2    | 1.95                     | 0.79              |
| 11:XK:32:ILE:CD1  | 11:XK:72:ALA:HB2   | 2.12                     | 0.79              |
| 27:YD:68:LYS:HB2  | 27:YD:70:TRP:CH2   | 2.17                     | 0.79              |
| 2:QB:35:GLU:O     | 2:QB:36:ARG:HD3    | 1.82                     | 0.79              |
| 3:QC:138:VAL:HG13 | 3:QC:149:ALA:HB1   | 1.64                     | 0.79              |
| 5:QE:10:MET:HB3   | 5:QE:32:VAL:HG22   | 1.63                     | 0.79              |
| 9:QI:19:LEU:HD23  | 9:QI:61:ALA:HB2    | 1.63                     | 0.79              |
| 25:RA:1454:U:OP1  | 37:RR:77:ARG:NH1   | 2.15                     | 0.79              |
| 1:XA:1055:A:O2'   | 3:XC:161:GLU:OE2   | 1.99                     | 0.79              |
| 2:XB:35:GLU:O     | 2:XB:36:ARG:HD3    | 1.82                     | 0.79              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:XE:10:MET:HB3    | 5:XE:32:VAL:HG22    | 1.63                     | 0.79              |
| 13:XM:4:ILE:H      | 13:XM:9:ILE:HG21    | 1.47                     | 0.79              |
| 27:YD:34:VAL:O     | 27:YD:34:VAL:HG13   | 1.81                     | 0.79              |
| 31:YH:150:ALA:C    | 31:YH:152:ARG:H     | 1.88                     | 0.79              |
| 16:QP:51:VAL:HG12  | 16:QP:52:ASP:N      | 1.97                     | 0.79              |
| 25:RA:1019:U:H3    | 25:RA:1142(A):A:H62 | 1.29                     | 0.79              |
| 27:RD:25:THR:CG2   | 27:RD:82:ILE:H      | 1.93                     | 0.79              |
| 28:RE:111:ARG:HE   | 28:RE:160:TYR:HE1   | 1.31                     | 0.79              |
| 30:RG:61:ALA:HB2   | 30:RG:68:PRO:CD     | 2.12                     | 0.79              |
| 30:RG:77:ILE:HD13  | 30:RG:82:LEU:HD12   | 1.64                     | 0.79              |
| 31:RH:10:PRO:O     | 31:RH:11:VAL:HG13   | 1.80                     | 0.79              |
| 2:XB:187:LEU:HA    | 2:XB:201:ILE:HB     | 1.65                     | 0.79              |
| 8:XH:100:ILE:HB    | 8:XH:125:ARG:HH12   | 1.47                     | 0.79              |
| 14:YN:40:CYS:SG    | 14:YN:43:CYS:HB2    | 2.21                     | 0.79              |
| 25:YA:2419:U:H5'   | 52:Y6:23:THR:HG22   | 1.64                     | 0.79              |
| 45:YZ:60:GLU:HA    | 45:YZ:66:SER:HA     | 1.64                     | 0.79              |
| 12:QL:11:VAL:HG13  | 17:QQ:29:HIS:CD2    | 2.17                     | 0.79              |
| 20:QT:89:ARG:HH21  | 20:QT:104:LEU:HD21  | 1.47                     | 0.79              |
| 27:RD:54:ARG:NH1   | 27:RD:54:ARG:HG3    | 1.98                     | 0.79              |
| 31:RH:126:PRO:CG   | 31:RH:127:GLU:H     | 1.96                     | 0.79              |
| 35:RP:14:LYS:O     | 35:RP:16:ARG:HG2    | 1.83                     | 0.79              |
| 36:RQ:81:VAL:O     | 36:RQ:82:ARG:CG     | 2.31                     | 0.79              |
| 39:RT:102:ILE:HA   | 39:RT:105:LEU:CD2   | 2.13                     | 0.79              |
| 1:XA:971:G:N2      | 1:XA:1363:A:OP2     | 2.13                     | 0.79              |
| 7:XG:89:MET:HE1    | 7:XG:156:TRP:H      | 1.47                     | 0.79              |
| 8:XH:20:TYR:HA     | 8:XH:65:TYR:CE2     | 2.18                     | 0.79              |
| 9:XI:15:ALA:HB2    | 9:XI:65:VAL:HG23    | 1.65                     | 0.79              |
| 12:XL:6:THR:N      | 12:XL:9:GLN:HE21    | 1.80                     | 0.79              |
| 25:YA:2573:C:N4    | 56:Z8:75:C:O2'      | 2.15                     | 0.79              |
| 31:YH:126:PRO:CG   | 31:YH:127:GLU:H     | 1.95                     | 0.79              |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:H     | 1.48                     | 0.79              |
| 36:YQ:81:VAL:O     | 36:YQ:82:ARG:CG     | 2.31                     | 0.79              |
| 39:YT:62:THR:CG2   | 39:YT:75:ILE:HG12   | 2.11                     | 0.79              |
| 40:YU:105:VAL:HG22 | 41:YV:44:LYS:HD2    | 1.65                     | 0.79              |
| 49:Y3:56:VAL:HG12  | 49:Y3:57:GLU:H      | 1.48                     | 0.79              |
| 12:QL:10:LEU:HD13  | 17:QQ:32:TYR:HE2    | 1.45                     | 0.79              |
| 12:QL:48:PRO:HD2   | 12:QL:49:ASN:N      | 1.97                     | 0.79              |
| 28:RE:137:HIS:HB3  | 28:RE:138:PRO:HD2   | 1.65                     | 0.79              |
| 39:YT:102:ILE:HA   | 39:YT:105:LEU:CD2   | 2.13                     | 0.79              |
| 35:RP:59:LEU:HA    | 35:RP:61:ARG:HH21   | 1.44                     | 0.79              |
| 12:XL:86:ARG:HB2   | 12:XL:101:VAL:HG22  | 1.62                     | 0.79              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:XR:43:PHE:HE2   | 18:XR:58:LEU:HD11 | 1.47                     | 0.79              |
| 19:XS:41:VAL:HG12  | 19:XS:44:MET:N    | 1.98                     | 0.79              |
| 30:YG:77:ILE:HD13  | 30:YG:82:LEU:HD12 | 1.65                     | 0.79              |
| 35:YP:14:LYS:O     | 35:YP:16:ARG:HG2  | 1.83                     | 0.79              |
| 35:YP:65:ARG:HG3   | 35:YP:65:ARG:NH1  | 1.90                     | 0.79              |
| 7:QG:89:MET:HE1    | 7:QG:156:TRP:H    | 1.47                     | 0.79              |
| 11:QK:124:LYS:HD2  | 11:QK:125:PHE:HE1 | 1.45                     | 0.79              |
| 19:QS:41:VAL:HG12  | 19:QS:44:MET:N    | 1.98                     | 0.79              |
| 31:RH:86:GLU:CG    | 31:RH:165:ALA:H   | 1.94                     | 0.79              |
| 34:RO:31:LYS:HG3   | 34:RO:32:TYR:CE2  | 2.17                     | 0.79              |
| 35:RP:97:PRO:O     | 35:RP:98:GLU:HB3  | 1.83                     | 0.79              |
| 4:XD:165:MET:HA    | 4:XD:165:MET:HE3  | 1.65                     | 0.79              |
| 18:XR:56:THR:HB    | 18:XR:58:LEU:CD1  | 2.13                     | 0.79              |
| 19:XS:5:LEU:HD11   | 50:Y4:66:SER:CB   | 2.12                     | 0.79              |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:H   | 1.48                     | 0.79              |
| 25:YA:602:G:HO2'   | 25:YA:604:G:HO2'  | 1.26                     | 0.79              |
| 27:YD:17:THR:CG2   | 27:YD:205:VAL:H   | 1.96                     | 0.79              |
| 31:YH:26:VAL:HG13  | 31:YH:27:LYS:N    | 1.96                     | 0.79              |
| 27:RD:68:LYS:HB2   | 27:RD:70:TRP:CH2  | 2.17                     | 0.79              |
| 33:RN:71:ILE:HG21  | 33:RN:84:LYS:HB3  | 1.65                     | 0.79              |
| 1:XA:1297:C:O2'    | 7:XG:114:ARG:NH2  | 2.16                     | 0.79              |
| 4:XD:28:SER:HB3    | 4:XD:29:PRO:HD2   | 1.65                     | 0.79              |
| 31:YH:150:ALA:O    | 31:YH:152:ARG:N   | 2.14                     | 0.79              |
| 31:YH:153:LYS:CG   | 31:YH:162:ILE:H   | 1.96                     | 0.79              |
| 35:YP:47:ASP:OD2   | 35:YP:49:ARG:HG2  | 1.82                     | 0.79              |
| 8:QH:20:TYR:HA     | 8:QH:65:TYR:CE2   | 2.18                     | 0.79              |
| 40:RU:105:VAL:HG22 | 41:RV:44:LYS:HD2  | 1.65                     | 0.79              |
| 25:YA:1454:U:H5'   | 37:YR:63:ARG:HE   | 1.45                     | 0.79              |
| 25:YA:1454:U:OP1   | 37:YR:77:ARG:NH1  | 2.15                     | 0.79              |
| 47:Y1:11:ARG:HB3   | 47:Y1:11:ARG:NH1  | 1.98                     | 0.79              |
| 12:QL:6:THR:N      | 12:QL:9:GLN:HE21  | 1.80                     | 0.78              |
| 13:XM:3:ARG:CA     | 13:XM:9:ILE:HG21  | 2.13                     | 0.78              |
| 13:XM:8:GLU:OE2    | 30:YG:115:ARG:NH1 | 2.16                     | 0.78              |
| 34:YO:53:LYS:HD2   | 34:YO:53:LYS:N    | 1.96                     | 0.78              |
| 50:Y4:58:ARG:O     | 50:Y4:63:TYR:HB2  | 1.84                     | 0.78              |
| 13:QM:4:ILE:H      | 13:QM:9:ILE:HG21  | 1.47                     | 0.78              |
| 18:QR:56:THR:HB    | 18:QR:58:LEU:CD1  | 2.13                     | 0.78              |
| 22:QV:75:C:OP1     | 25:RA:2602:A:OP1  | 2.01                     | 0.78              |
| 33:RN:43:THR:HB    | 33:RN:46:VAL:HG12 | 1.63                     | 0.78              |
| 33:RN:62:VAL:HG12  | 33:RN:66:LYS:HD2  | 1.65                     | 0.78              |
| 1:XA:973:G:O3'     | 14:YN:41:ARG:NH1  | 2.17                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:XI:83:ARG:O      | 9:XI:86:VAL:HG12   | 1.84                     | 0.78              |
| 27:YD:27:THR:HG21  | 27:YD:83:GLU:HB3   | 1.63                     | 0.78              |
| 40:YU:90:VAL:HG12  | 40:YU:91:ASP:N     | 1.98                     | 0.78              |
| 44:YY:86:ARG:HB2   | 44:YY:95:LYS:HD2   | 1.65                     | 0.78              |
| 2:QB:84:GLU:HB3    | 2:QB:219:VAL:HG21  | 1.65                     | 0.78              |
| 4:QD:30:LYS:HD3    | 4:QD:30:LYS:N      | 1.98                     | 0.78              |
| 9:QI:15:ALA:HB2    | 9:QI:65:VAL:HG23   | 1.65                     | 0.78              |
| 36:RQ:80:GLU:O     | 36:RQ:81:VAL:CG1   | 2.30                     | 0.78              |
| 43:RX:70:LEU:HD23  | 43:RX:70:LEU:N     | 1.99                     | 0.78              |
| 47:R1:11:ARG:NH1   | 47:R1:11:ARG:HB3   | 1.98                     | 0.78              |
| 4:QD:28:SER:HB2    | 4:QD:29:PRO:CD     | 2.14                     | 0.78              |
| 27:RD:54:ARG:HG3   | 27:RD:54:ARG:HH11  | 1.49                     | 0.78              |
| 10:XJ:16:LEU:HD23  | 10:XJ:94:VAL:HG13  | 1.66                     | 0.78              |
| 36:YQ:59:ARG:HD3   | 36:YQ:59:ARG:H     | 1.48                     | 0.78              |
| 1:QA:1139:G:N2     | 1:QA:1143:G:O6     | 2.15                     | 0.78              |
| 3:QC:181:ASN:ND2   | 3:QC:204:LEU:HD12  | 1.99                     | 0.78              |
| 10:QJ:40:LEU:HB2   | 10:QJ:69:ASN:HB3   | 1.65                     | 0.78              |
| 11:QK:32:ILE:CD1   | 11:QK:72:ALA:HB2   | 2.12                     | 0.78              |
| 18:QR:43:PHE:HE2   | 18:QR:58:LEU:HD11  | 1.47                     | 0.78              |
| 20:QT:50:GLU:HG3   | 20:QT:51:GLU:N     | 1.97                     | 0.78              |
| 29:RF:20:LEU:HD12  | 29:RF:21:ALA:H     | 1.48                     | 0.78              |
| 30:RG:61:ALA:HB2   | 30:RG:68:PRO:HD3   | 1.65                     | 0.78              |
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:HG2  | 1.48                     | 0.78              |
| 13:XM:88:ARG:HH11  | 13:XM:88:ARG:CB    | 1.95                     | 0.78              |
| 30:YG:128:ARG:HH21 | 30:YG:128:ARG:HG3  | 1.48                     | 0.78              |
| 34:YO:97:ARG:H     | 34:YO:117:LEU:HD22 | 1.48                     | 0.78              |
| 41:YV:47:VAL:HG13  | 41:YV:48:GLY:H     | 1.49                     | 0.78              |
| 43:YX:70:LEU:HD23  | 43:YX:70:LEU:N     | 1.99                     | 0.78              |
| 4:QD:165:MET:HA    | 4:QD:165:MET:HE3   | 1.65                     | 0.78              |
| 25:RA:1454:U:H5'   | 37:RR:63:ARG:HE    | 1.48                     | 0.78              |
| 36:RQ:20:ALA:HB1   | 36:RQ:99:PRO:HB2   | 1.65                     | 0.78              |
| 40:RU:90:VAL:HG12  | 40:RU:91:ASP:N     | 1.97                     | 0.78              |
| 49:R3:56:VAL:HG12  | 49:R3:57:GLU:H     | 1.48                     | 0.78              |
| 19:XS:5:LEU:HD22   | 50:Y4:67:TYR:CE2   | 2.19                     | 0.78              |
| 27:YD:54:ARG:HG3   | 27:YD:54:ARG:NH1   | 1.98                     | 0.78              |
| 27:YD:94:LEU:HD22  | 27:YD:95:LEU:N     | 1.98                     | 0.78              |
| 7:QG:113:GLU:HB2   | 7:QG:119:ARG:HG2   | 1.66                     | 0.78              |
| 31:RH:153:LYS:CG   | 31:RH:162:ILE:H    | 1.96                     | 0.78              |
| 25:YA:958:U:OP2    | 36:YQ:14:ARG:NH1   | 2.16                     | 0.78              |
| 28:YE:4:ILE:HD12   | 28:YE:28:ALA:HB1   | 1.66                     | 0.78              |
| 29:YF:145:GLU:O    | 29:YF:145:GLU:HG3  | 1.81                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:448:A:OP2     | 1:QA:485:G:N2      | 2.17                     | 0.78              |
| 34:RO:47:ILE:HD12  | 34:RO:48:PRO:HD2   | 1.66                     | 0.78              |
| 44:RY:86:ARG:HB2   | 44:RY:95:LYS:HD2   | 1.64                     | 0.78              |
| 3:XC:138:VAL:HG13  | 3:XC:149:ALA:HB1   | 1.64                     | 0.78              |
| 28:YE:137:HIS:HB3  | 28:YE:138:PRO:HD2  | 1.65                     | 0.78              |
| 35:YP:19:VAL:HG22  | 35:YP:20:GLY:N     | 1.97                     | 0.78              |
| 2:QB:18:GLY:H      | 2:QB:42:ILE:CG2    | 1.95                     | 0.78              |
| 20:QT:100:ILE:HG13 | 20:QT:102:GLY:H    | 1.48                     | 0.78              |
| 27:RD:94:LEU:HD22  | 27:RD:95:LEU:N     | 1.98                     | 0.78              |
| 27:YD:34:VAL:HG21  | 27:YD:103:ARG:HA   | 1.66                     | 0.78              |
| 2:QB:101:MET:CA    | 2:QB:108:ILE:HG13  | 2.11                     | 0.78              |
| 5:QE:11:ILE:CD1    | 5:QE:31:LEU:HD12   | 2.13                     | 0.78              |
| 27:RD:142:VAL:HG23 | 27:RD:193:VAL:HA   | 1.66                     | 0.78              |
| 28:RE:24:THR:HG21  | 28:RE:188:VAL:CG1  | 2.13                     | 0.78              |
| 29:RF:29:ASN:H     | 29:RF:112:MET:CE   | 1.97                     | 0.78              |
| 35:RP:75:ILE:HD13  | 35:RP:75:ILE:N     | 1.99                     | 0.78              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:HD21 | 1.64                     | 0.78              |
| 6:XF:24:GLU:HA     | 6:XF:27:GLN:CG     | 2.14                     | 0.78              |
| 30:YG:97:ASP:H     | 30:YG:100:TRP:HD1  | 1.31                     | 0.78              |
| 31:YH:132:ARG:HB2  | 31:YH:132:ARG:NH1  | 1.94                     | 0.78              |
| 1:QA:1347:G:N2     | 1:QA:1374:A:OP2    | 2.15                     | 0.77              |
| 10:QJ:16:LEU:HD23  | 10:QJ:94:VAL:HG13  | 1.66                     | 0.77              |
| 28:RE:4:ILE:HD12   | 28:RE:28:ALA:HB1   | 1.66                     | 0.77              |
| 40:RU:66:ASN:O     | 40:RU:70:ARG:HB2   | 1.84                     | 0.77              |
| 7:XG:113:GLU:HB2   | 7:XG:119:ARG:HG2   | 1.65                     | 0.77              |
| 25:YA:1021:A:N6    | 25:YA:1141:U:O2    | 2.17                     | 0.77              |
| 28:YE:24:THR:HG21  | 28:YE:188:VAL:CG1  | 2.13                     | 0.77              |
| 38:YS:106:ARG:HA   | 38:YS:110:LEU:HD21 | 1.64                     | 0.77              |
| 40:YU:66:ASN:O     | 40:YU:70:ARG:HB2   | 1.84                     | 0.77              |
| 6:QF:24:GLU:HA     | 6:QF:27:GLN:CG     | 2.14                     | 0.77              |
| 22:QV:56:C:O2'     | 30:RG:78:SER:HB2   | 1.83                     | 0.77              |
| 25:RA:2580:U:H4'   | 28:RE:130:GLY:HA3  | 1.66                     | 0.77              |
| 27:RD:25:THR:O     | 27:RD:27:THR:N     | 2.18                     | 0.77              |
| 30:RG:128:ARG:HH21 | 30:RG:128:ARG:HG3  | 1.48                     | 0.77              |
| 2:XB:239:VAL:HG12  | 2:XB:240:GLN:NE2   | 1.99                     | 0.77              |
| 25:YA:587:C:OP2    | 35:YP:21:ARG:NH2   | 2.18                     | 0.77              |
| 31:YH:152:ARG:HG3  | 31:YH:153:LYS:CE   | 2.13                     | 0.77              |
| 33:YN:71:ILE:HG21  | 33:YN:84:LYS:HB3   | 1.65                     | 0.77              |
| 34:YO:47:ILE:HD12  | 34:YO:48:PRO:HD2   | 1.67                     | 0.77              |
| 2:QB:44:LEU:HD12   | 2:QB:44:LEU:H      | 1.48                     | 0.77              |
| 4:QD:9:CYS:SG      | 4:QD:22:LYS:HD2    | 2.25                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:17:THR:CG2   | 27:RD:205:VAL:H    | 1.96                     | 0.77              |
| 35:RP:62:LEU:N     | 35:RP:62:LEU:CD2   | 2.46                     | 0.77              |
| 1:XA:1314:C:OP2    | 19:XS:4:SER:OG     | 2.02                     | 0.77              |
| 9:XI:53:VAL:HB     | 9:XI:95:LYS:HE3    | 1.66                     | 0.77              |
| 13:XM:15:VAL:HG23  | 13:XM:43:THR:O     | 1.84                     | 0.77              |
| 27:YD:25:THR:HG22  | 27:YD:82:ILE:H     | 1.46                     | 0.77              |
| 35:YP:84:ASN:ND2   | 35:YP:116:GLY:HA3  | 1.99                     | 0.77              |
| 2:QB:122:PHE:HD1   | 2:QB:139:LYS:HZ1   | 1.30                     | 0.77              |
| 2:QB:239:VAL:HG12  | 2:QB:240:GLN:NE2   | 1.99                     | 0.77              |
| 6:QF:23:LYS:O      | 6:QF:27:GLN:HG2    | 1.85                     | 0.77              |
| 8:QH:100:ILE:HB    | 8:QH:125:ARG:HH12  | 1.47                     | 0.77              |
| 17:QQ:41:LYS:NZ    | 17:QQ:92:ARG:HH22  | 1.82                     | 0.77              |
| 28:RE:55:ASN:C     | 28:RE:57:LYS:H     | 1.91                     | 0.77              |
| 31:RH:150:ALA:O    | 31:RH:152:ARG:N    | 2.14                     | 0.77              |
| 35:RP:84:ASN:ND2   | 35:RP:116:GLY:HA3  | 1.99                     | 0.77              |
| 35:RP:114:ILE:HD11 | 35:RP:130:PHE:CE1  | 2.19                     | 0.77              |
| 39:RT:43:GLN:HG2   | 39:RT:44:ASP:N     | 1.99                     | 0.77              |
| 42:RW:65:LEU:CD1   | 42:RW:68:ARG:HH11  | 1.97                     | 0.77              |
| 44:RY:97:ARG:HH21  | 44:RY:98:VAL:CB    | 1.98                     | 0.77              |
| 2:XB:84:GLU:HB3    | 2:XB:219:VAL:HG21  | 1.65                     | 0.77              |
| 25:YA:2014:A:O2'   | 51:Y5:2:ALA:HB2    | 1.85                     | 0.77              |
| 29:YF:20:LEU:HD12  | 29:YF:21:ALA:H     | 1.49                     | 0.77              |
| 37:YR:74:LYS:O     | 37:YR:75:LEU:HB3   | 1.84                     | 0.77              |
| 38:YS:83:LYS:C     | 38:YS:109:GLY:HA3  | 2.09                     | 0.77              |
| 5:QE:12:LEU:HD23   | 5:QE:13:ILE:N      | 2.00                     | 0.77              |
| 25:RA:993:G:OP1    | 40:RU:50:ARG:NH2   | 2.18                     | 0.77              |
| 50:R4:22:ILE:O     | 50:R4:24:THR:HG23  | 1.84                     | 0.77              |
| 16:XP:72:ARG:HD3   | 16:XP:72:ARG:C     | 2.10                     | 0.77              |
| 25:YA:1689:A:H62   | 25:YA:1698:A:H2    | 1.30                     | 0.77              |
| 35:YP:88:LEU:C     | 35:YP:90:ARG:H     | 1.92                     | 0.77              |
| 47:Y1:13:ILE:HD11  | 47:Y1:42:GLN:OE1   | 1.84                     | 0.77              |
| 25:YA:242:G:H5'    | 54:Y8:62:LEU:HD22  | 1.67                     | 0.77              |
| 28:YE:55:ASN:C     | 28:YE:57:LYS:H     | 1.91                     | 0.77              |
| 29:YF:11:VAL:HB    | 29:YF:18:ARG:HG3   | 1.64                     | 0.77              |
| 50:Y4:22:ILE:O     | 50:Y4:24:THR:HG23  | 1.84                     | 0.77              |
| 51:Y5:40:LYS:CD    | 51:Y5:46:CYS:HB3   | 2.15                     | 0.77              |
| 54:Y8:59:LYS:CB    | 54:Y8:59:LYS:HZ3   | 1.96                     | 0.77              |
| 17:QQ:59:ILE:H     | 17:QQ:59:ILE:HD13  | 1.50                     | 0.77              |
| 25:RA:2404:C:O3'   | 35:RP:77:ARG:NH2   | 2.17                     | 0.77              |
| 27:RD:146:GLU:HB2  | 27:RD:189:CYS:HB3  | 1.67                     | 0.77              |
| 35:RP:127:ALA:C    | 35:RP:147:LEU:HD23 | 2.10                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:RS:60:GLY:O     | 38:RS:61:ASN:HB3   | 1.84                     | 0.77              |
| 47:R1:86:SER:N     | 47:R1:87:PRO:CD    | 2.48                     | 0.77              |
| 1:XA:1189:C:OP1    | 10:XJ:51:ARG:NH2   | 2.18                     | 0.77              |
| 27:YD:44:ASN:HD22  | 27:YD:44:ASN:N     | 1.79                     | 0.77              |
| 44:YY:79:CYS:SG    | 44:YY:80:GLY:N     | 2.57                     | 0.77              |
| 4:QD:76:ARG:HD2    | 4:QD:207:TYR:CE2   | 2.20                     | 0.77              |
| 34:RO:97:ARG:H     | 34:RO:117:LEU:HD22 | 1.48                     | 0.77              |
| 2:XB:44:LEU:H      | 2:XB:44:LEU:HD12   | 1.48                     | 0.77              |
| 5:XE:42:GLY:HA3    | 5:XE:66:MET:HG2    | 1.67                     | 0.77              |
| 19:XS:39:THR:HG22  | 19:XS:40:ILE:H     | 1.50                     | 0.77              |
| 25:YA:1187:G:H5''  | 41:YV:81:TYR:CE2   | 2.19                     | 0.77              |
| 29:YF:183:VAL:O    | 29:YF:187:VAL:HG23 | 1.85                     | 0.77              |
| 36:YQ:20:ALA:CB    | 36:YQ:99:PRO:HD2   | 2.14                     | 0.77              |
| 36:YQ:79:LEU:HD22  | 36:YQ:79:LEU:C     | 2.07                     | 0.77              |
| 42:YW:65:LEU:CD1   | 42:YW:68:ARG:HH11  | 1.97                     | 0.77              |
| 16:QP:6:LEU:HB3    | 16:QP:17:TYR:HD2   | 1.50                     | 0.77              |
| 31:RH:153:LYS:HA   | 31:RH:153:LYS:NZ   | 1.99                     | 0.77              |
| 35:RP:88:LEU:C     | 35:RP:90:ARG:H     | 1.92                     | 0.77              |
| 36:RQ:79:LEU:HD22  | 36:RQ:79:LEU:C     | 2.07                     | 0.77              |
| 44:RY:79:CYS:SG    | 44:RY:80:GLY:N     | 2.57                     | 0.77              |
| 47:R1:13:ILE:HD11  | 47:R1:42:GLN:OE1   | 1.84                     | 0.77              |
| 1:XA:1129:C:H4'    | 1:XA:1130:A:H5'    | 1.67                     | 0.77              |
| 6:XF:23:LYS:O      | 6:XF:27:GLN:HG2    | 1.84                     | 0.77              |
| 20:XT:13:LEU:HD12  | 20:XT:14:LYS:N     | 2.00                     | 0.77              |
| 20:XT:89:ARG:HH21  | 20:XT:104:LEU:HD21 | 1.47                     | 0.77              |
| 25:YA:2131:G:H4'   | 25:YA:2132:U:H4'   | 1.66                     | 0.77              |
| 26:YB:42:C:H42     | 30:YG:91:ARG:HH21  | 1.31                     | 0.77              |
| 48:Y2:47:ASN:H     | 48:Y2:47:ASN:HD22  | 1.33                     | 0.77              |
| 49:Y3:35:ARG:HB3   | 49:Y3:37:LEU:HD21  | 1.66                     | 0.77              |
| 31:RH:26:VAL:HG13  | 31:RH:27:LYS:N     | 1.96                     | 0.77              |
| 39:RT:57:PHE:C     | 39:RT:58:ASN:HD22  | 1.93                     | 0.77              |
| 50:R4:1:MET:HB2    | 50:R4:6:HIS:NE2    | 2.00                     | 0.77              |
| 50:R4:58:ARG:O     | 50:R4:63:TYR:HB2   | 1.84                     | 0.77              |
| 5:XE:11:ILE:CD1    | 5:XE:31:LEU:HD12   | 2.13                     | 0.77              |
| 27:YD:25:THR:O     | 27:YD:27:THR:N     | 2.17                     | 0.77              |
| 27:YD:153:ALA:O    | 27:YD:154:LYS:HG3  | 1.85                     | 0.77              |
| 36:YQ:119:ARG:HH11 | 36:YQ:119:ARG:HG2  | 1.48                     | 0.77              |
| 42:YW:18:ARG:HG3   | 42:YW:76:VAL:CG1   | 2.16                     | 0.77              |
| 13:QM:88:ARG:HH11  | 13:QM:88:ARG:CB    | 1.96                     | 0.76              |
| 20:QT:26:ASN:O     | 20:QT:30:LYS:HB2   | 1.86                     | 0.76              |
| 25:RA:1252:G:N3    | 40:RU:33:ARG:HD2   | 2.00                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2111:C:N3    | 25:RA:2118:U:O2'   | 2.18                     | 0.76              |
| 25:RA:2810:A:O3'   | 28:RE:61:ARG:HG3   | 1.85                     | 0.76              |
| 27:RD:44:ASN:HD22  | 27:RD:44:ASN:N     | 1.79                     | 0.76              |
| 29:RF:183:VAL:O    | 29:RF:187:VAL:HG23 | 1.85                     | 0.76              |
| 44:RY:97:ARG:NH2   | 44:RY:98:VAL:HB    | 2.00                     | 0.76              |
| 11:XK:77:MET:HE3   | 11:XK:80:VAL:HG12  | 1.67                     | 0.76              |
| 31:YH:153:LYS:HA   | 31:YH:153:LYS:NZ   | 1.99                     | 0.76              |
| 35:YP:114:ILE:HD11 | 35:YP:130:PHE:CE1  | 2.19                     | 0.76              |
| 35:YP:127:ALA:C    | 35:YP:147:LEU:HD23 | 2.10                     | 0.76              |
| 50:Y4:1:MET:HB2    | 50:Y4:6:HIS:NE2    | 2.00                     | 0.76              |
| 54:Y8:60:LEU:C     | 54:Y8:63:PRO:HD2   | 2.11                     | 0.76              |
| 2:QB:187:LEU:HA    | 2:QB:201:ILE:HB    | 1.65                     | 0.76              |
| 37:RR:33:ARG:HH22  | 51:R5:55:ARG:HG2   | 1.51                     | 0.76              |
| 4:XD:76:ARG:HD2    | 4:XD:207:TYR:CE2   | 2.20                     | 0.76              |
| 14:XN:25:VAL:HG22  | 14:XN:38:GLY:O     | 1.84                     | 0.76              |
| 28:YE:111:ARG:HE   | 28:YE:160:TYR:HE1  | 1.31                     | 0.76              |
| 33:YN:62:VAL:HG12  | 33:YN:66:LYS:HD2   | 1.65                     | 0.76              |
| 34:YO:104:ARG:HH11 | 34:YO:104:ARG:HG2  | 1.50                     | 0.76              |
| 36:YQ:59:ARG:H     | 36:YQ:59:ARG:CD    | 1.99                     | 0.76              |
| 21:QU:10:ARG:HG2   | 21:QU:13:ILE:HD12  | 1.68                     | 0.76              |
| 25:RA:1803:A:H4'   | 27:RD:259:THR:CG2  | 2.15                     | 0.76              |
| 29:RF:32:LEU:C     | 29:RF:32:LEU:HD12  | 2.10                     | 0.76              |
| 30:RG:127:GLY:O    | 30:RG:128:ARG:HG2  | 1.85                     | 0.76              |
| 36:RQ:20:ALA:CB    | 36:RQ:99:PRO:HD2   | 2.14                     | 0.76              |
| 36:RQ:66:ILE:HG13  | 36:RQ:67:ARG:N     | 1.99                     | 0.76              |
| 36:RQ:90:VAL:HG13  | 36:RQ:91:GLU:H     | 1.49                     | 0.76              |
| 40:RU:88:ILE:HG22  | 40:RU:90:VAL:HG23  | 1.67                     | 0.76              |
| 4:XD:20:TYR:CD2    | 4:XD:27:TYR:HE2    | 2.01                     | 0.76              |
| 5:XE:53:LEU:H      | 5:XE:53:LEU:CD1    | 1.99                     | 0.76              |
| 7:XG:79:ARG:HH22   | 7:XG:82:GLY:HA2    | 1.51                     | 0.76              |
| 25:YA:498:G:N3     | 44:YY:47:LYS:NZ    | 2.32                     | 0.76              |
| 29:YF:32:LEU:C     | 29:YF:32:LEU:HD12  | 2.10                     | 0.76              |
| 36:YQ:66:ILE:HG13  | 36:YQ:67:ARG:N     | 1.99                     | 0.76              |
| 38:YS:60:GLY:O     | 38:YS:61:ASN:HB3   | 1.84                     | 0.76              |
| 44:YY:94:LYS:O     | 44:YY:101:LYS:HB3  | 1.85                     | 0.76              |
| 47:Y1:80:LEU:C     | 47:Y1:81:LYS:HE2   | 2.10                     | 0.76              |
| 1:QA:1189:C:OP1    | 10:QJ:51:ARG:NH2   | 2.18                     | 0.76              |
| 7:QG:148:ASN:HD22  | 7:QG:148:ASN:N     | 1.82                     | 0.76              |
| 4:XD:9:CYS:SG      | 4:XD:22:LYS:HD2    | 2.25                     | 0.76              |
| 36:YQ:20:ALA:HB1   | 36:YQ:99:PRO:HB2   | 1.65                     | 0.76              |
| 4:QD:13:ARG:CA     | 4:QD:33:MET:HE3    | 2.16                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:QI:83:ARG:O      | 9:QI:86:VAL:HG12   | 1.84                     | 0.76              |
| 20:QT:13:LEU:HD12  | 20:QT:14:LYS:N     | 2.00                     | 0.76              |
| 27:RD:34:VAL:HG21  | 27:RD:103:ARG:HA   | 1.66                     | 0.76              |
| 30:RG:101:ILE:HG13 | 30:RG:102:PHE:H    | 1.49                     | 0.76              |
| 44:RY:81:LYS:HD3   | 44:RY:97:ARG:NE    | 2.00                     | 0.76              |
| 49:R3:35:ARG:HB3   | 49:R3:37:LEU:HD21  | 1.66                     | 0.76              |
| 52:R6:34:LEU:HD13  | 52:R6:34:LEU:H     | 1.50                     | 0.76              |
| 3:XC:59:ARG:HH22   | 3:XC:97:LYS:HE3    | 1.51                     | 0.76              |
| 30:YG:61:ALA:HB2   | 30:YG:68:PRO:HD3   | 1.65                     | 0.76              |
| 30:YG:127:GLY:O    | 30:YG:128:ARG:HG2  | 1.85                     | 0.76              |
| 30:YG:142:PRO:HB2  | 50:Y4:31:ILE:HD13  | 1.68                     | 0.76              |
| 13:QM:15:VAL:HG23  | 13:QM:43:THR:O     | 1.84                     | 0.76              |
| 19:QS:68:GLY:CA    | 50:R4:68:ARG:HG2   | 2.16                     | 0.76              |
| 55:R9:1:MET:HB3    | 55:R9:4:ARG:NH1    | 2.01                     | 0.76              |
| 2:XB:4:GLU:HG2     | 2:XB:5:ILE:N       | 1.95                     | 0.76              |
| 9:XI:113:LYS:HD2   | 9:XI:113:LYS:H     | 1.51                     | 0.76              |
| 48:Y2:41:ILE:C     | 48:Y2:41:ILE:HD12  | 2.10                     | 0.76              |
| 4:QD:153:ARG:NH1   | 4:QD:181:MET:HG3   | 2.00                     | 0.76              |
| 5:QE:72:GLN:NE2    | 5:QE:144:THR:HG22  | 2.01                     | 0.76              |
| 27:RD:153:ALA:O    | 27:RD:154:LYS:HG3  | 1.85                     | 0.76              |
| 7:XG:37:ASN:ND2    | 9:XI:40:LEU:HD23   | 2.00                     | 0.76              |
| 29:YF:29:ASN:H     | 29:YF:112:MET:CE   | 1.98                     | 0.76              |
| 31:YH:125:VAL:HA   | 31:YH:126:PRO:HB3  | 1.68                     | 0.76              |
| 36:YQ:90:VAL:HG13  | 36:YQ:91:GLU:H     | 1.49                     | 0.76              |
| 3:QC:59:ARG:HH22   | 3:QC:97:LYS:HE3    | 1.50                     | 0.76              |
| 5:QE:42:GLY:HA3    | 5:QE:66:MET:HG2    | 1.68                     | 0.76              |
| 16:QP:22:THR:HA    | 16:QP:33:ILE:HG12  | 1.66                     | 0.76              |
| 27:RD:69:ARG:HH21  | 27:RD:130:ALA:CB   | 1.99                     | 0.76              |
| 10:XJ:38:ILE:HG12  | 10:XJ:71:LEU:O     | 1.86                     | 0.76              |
| 27:YD:69:ARG:HH21  | 27:YD:130:ALA:CB   | 1.99                     | 0.76              |
| 30:YG:76:SER:OG    | 30:YG:83:ARG:HA    | 1.85                     | 0.76              |
| 42:YW:73:ALA:HB3   | 42:YW:106:ILE:HG12 | 1.68                     | 0.76              |
| 44:YY:81:LYS:HD3   | 44:YY:97:ARG:NE    | 2.01                     | 0.76              |
| 8:QH:5:PRO:O       | 8:QH:8:ASP:HB3     | 1.86                     | 0.76              |
| 16:QP:72:ARG:HD3   | 16:QP:72:ARG:C     | 2.10                     | 0.76              |
| 47:R1:56:GLN:NE2   | 47:R1:56:GLN:N     | 2.34                     | 0.76              |
| 2:XB:117:GLU:O     | 2:XB:121:LEU:HB2   | 1.85                     | 0.76              |
| 5:XE:12:LEU:HD23   | 5:XE:13:ILE:N      | 2.00                     | 0.76              |
| 5:XE:36:ASP:OD2    | 5:XE:38:GLN:HB2    | 1.86                     | 0.76              |
| 17:XQ:41:LYS:NZ    | 17:XQ:92:ARG:HH22  | 1.82                     | 0.76              |
| 28:YE:36:ARG:HH21  | 28:YE:88:GLY:HA2   | 1.50                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:50:ILE:HD12  | 39:YT:102:ILE:HD11 | 1.68                     | 0.76              |
| 39:YT:111:ARG:O    | 39:YT:113:LYS:N    | 2.17                     | 0.76              |
| 44:YY:95:LYS:HB3   | 44:YY:100:ALA:CA   | 2.10                     | 0.76              |
| 4:QD:13:ARG:HA     | 4:QD:33:MET:HE3    | 1.67                     | 0.76              |
| 10:QJ:38:ILE:HG12  | 10:QJ:71:LEU:O     | 1.86                     | 0.76              |
| 25:RA:958:U:OP2    | 36:RQ:14:ARG:NH1   | 2.18                     | 0.76              |
| 30:RG:76:SER:OG    | 30:RG:83:ARG:HA    | 1.85                     | 0.76              |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:H    | 1.48                     | 0.76              |
| 50:R4:34:GLU:HG3   | 50:R4:35:VAL:H     | 1.51                     | 0.76              |
| 54:R8:60:LEU:C     | 54:R8:63:PRO:HD2   | 2.11                     | 0.76              |
| 1:XA:1152:A:OP1    | 10:XJ:68:HIS:NE2   | 2.19                     | 0.76              |
| 16:XP:51:VAL:HG12  | 16:XP:52:ASP:N     | 1.97                     | 0.76              |
| 34:YO:107:ARG:HA   | 34:YO:112:MET:HE1  | 1.67                     | 0.76              |
| 35:YP:97:PRO:O     | 35:YP:98:GLU:HB3   | 1.83                     | 0.76              |
| 50:Y4:34:GLU:HG3   | 50:Y4:35:VAL:H     | 1.51                     | 0.76              |
| 52:Y6:34:LEU:H     | 52:Y6:34:LEU:HD13  | 1.50                     | 0.76              |
| 5:QE:53:LEU:H      | 5:QE:53:LEU:CD1    | 1.99                     | 0.75              |
| 6:QF:91:VAL:HG13   | 18:QR:72:ARG:HH12  | 1.51                     | 0.75              |
| 18:QR:53:ARG:HH21  | 18:QR:60:ALA:N     | 1.84                     | 0.75              |
| 25:RA:2324:C:H5''  | 25:RA:2325:G:H5''  | 1.68                     | 0.75              |
| 34:RO:104:ARG:HH11 | 34:RO:104:ARG:HG2  | 1.50                     | 0.75              |
| 37:RR:74:LYS:O     | 37:RR:75:LEU:HB3   | 1.84                     | 0.75              |
| 38:RS:83:LYS:C     | 38:RS:109:GLY:HA3  | 2.10                     | 0.75              |
| 40:RU:52:ARG:HH11  | 40:RU:52:ARG:HG2   | 1.50                     | 0.75              |
| 25:YA:1190:G:OP1   | 35:YP:30:THR:OG1   | 2.04                     | 0.75              |
| 28:YE:63:LEU:CD1   | 28:YE:65:GLY:H     | 1.99                     | 0.75              |
| 35:YP:62:LEU:N     | 35:YP:62:LEU:CD2   | 2.46                     | 0.75              |
| 40:YU:88:ILE:HG22  | 40:YU:90:VAL:HG23  | 1.67                     | 0.75              |
| 44:YY:44:ILE:HG13  | 44:YY:45:VAL:N     | 1.99                     | 0.75              |
| 47:Y1:86:SER:N     | 47:Y1:87:PRO:CD    | 2.48                     | 0.75              |
| 9:QI:53:VAL:HB     | 9:QI:95:LYS:HE3    | 1.67                     | 0.75              |
| 14:QN:22:THR:O     | 14:QN:23:ARG:HB2   | 1.86                     | 0.75              |
| 29:RF:129:PHE:HA   | 29:RF:142:TRP:NE1  | 2.02                     | 0.75              |
| 51:R5:40:LYS:CD    | 51:R5:46:CYS:HB3   | 2.15                     | 0.75              |
| 51:R5:47:PRO:O     | 51:R5:48:GLU:HG3   | 1.86                     | 0.75              |
| 1:XA:375:U:H4'     | 16:XP:17:TYR:HE2   | 1.51                     | 0.75              |
| 9:XI:62:TYR:C      | 9:XI:63:ILE:HD12   | 2.12                     | 0.75              |
| 10:XJ:40:LEU:HB2   | 10:XJ:69:ASN:HB3   | 1.65                     | 0.75              |
| 16:XP:6:LEU:HB3    | 16:XP:17:TYR:HD2   | 1.50                     | 0.75              |
| 29:YF:101:LEU:CD1  | 29:YF:102:PRO:HD2  | 2.12                     | 0.75              |
| 30:YG:3:LEU:HD12   | 30:YG:4:ASP:H      | 1.52                     | 0.75              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:YO:47:ILE:CD1   | 34:YO:48:PRO:HD2    | 2.16                     | 0.75              |
| 43:YX:57:LEU:HD11  | 43:YX:78:LYS:HB2    | 1.67                     | 0.75              |
| 47:Y1:81:LYS:NZ    | 47:Y1:81:LYS:CA     | 2.30                     | 0.75              |
| 54:Y8:59:LYS:HB2   | 54:Y8:59:LYS:HZ2    | 1.49                     | 0.75              |
| 5:QE:11:ILE:HD11   | 5:QE:31:LEU:CD1     | 2.16                     | 0.75              |
| 25:RA:1689:A:H62   | 25:RA:1698:A:H2     | 1.32                     | 0.75              |
| 31:RH:152:ARG:HG3  | 31:RH:153:LYS:CE    | 2.14                     | 0.75              |
| 8:XH:5:PRO:O       | 8:XH:8:ASP:HB3      | 1.85                     | 0.75              |
| 25:YA:1019:U:H3    | 25:YA:1142(A):A:H62 | 1.32                     | 0.75              |
| 27:YD:142:VAL:HG23 | 27:YD:193:VAL:HA    | 1.66                     | 0.75              |
| 28:YE:23:VAL:HG21  | 28:YE:183:LEU:HD23  | 1.69                     | 0.75              |
| 40:YU:92:ARG:HH11  | 40:YU:95:LEU:CD1    | 2.00                     | 0.75              |
| 41:YV:52:VAL:HG21  | 41:YV:55:ALA:HB3    | 1.68                     | 0.75              |
| 55:Y9:1:MET:HB3    | 55:Y9:4:ARG:NH1     | 2.01                     | 0.75              |
| 2:QB:117:GLU:O     | 2:QB:121:LEU:HB2    | 1.86                     | 0.75              |
| 7:QG:37:ASN:ND2    | 9:QI:40:LEU:HD23    | 2.00                     | 0.75              |
| 26:RB:56:G:OP1     | 30:RG:27:ASN:ND2    | 2.20                     | 0.75              |
| 30:RG:3:LEU:HD12   | 30:RG:4:ASP:H       | 1.52                     | 0.75              |
| 35:RP:62:LEU:HD21  | 54:R8:25:MET:HB2    | 1.69                     | 0.75              |
| 16:XP:22:THR:HA    | 16:XP:33:ILE:HG12   | 1.66                     | 0.75              |
| 18:XR:53:ARG:HH21  | 18:XR:60:ALA:N      | 1.84                     | 0.75              |
| 25:YA:571:A:O2'    | 41:YV:78:LYS:NZ     | 2.20                     | 0.75              |
| 47:Y1:56:GLN:NE2   | 47:Y1:56:GLN:N      | 2.34                     | 0.75              |
| 5:QE:45:PHE:CE2    | 5:QE:47:LYS:HD2     | 2.22                     | 0.75              |
| 8:QH:91:ARG:HH11   | 8:QH:91:ARG:HG2     | 1.52                     | 0.75              |
| 12:QL:48:PRO:HD2   | 12:QL:49:ASN:H      | 1.52                     | 0.75              |
| 20:QT:58:LYS:HE3   | 20:QT:62:LEU:HD11   | 1.69                     | 0.75              |
| 30:RG:142:PRO:HB2  | 50:R4:31:ILE:HD13   | 1.68                     | 0.75              |
| 44:RY:94:LYS:O     | 44:RY:101:LYS:HB3   | 1.85                     | 0.75              |
| 13:XM:49:THR:HG22  | 13:XM:51:ALA:N      | 2.01                     | 0.75              |
| 16:XP:43:LYS:HG2   | 16:XP:48:TRP:CE3    | 2.22                     | 0.75              |
| 30:YG:101:ILE:HG13 | 30:YG:102:PHE:H     | 1.49                     | 0.75              |
| 35:YP:62:LEU:HD21  | 54:Y8:25:MET:HB2    | 1.69                     | 0.75              |
| 10:QJ:27:ALA:HB1   | 10:QJ:34:VAL:HG21   | 1.69                     | 0.75              |
| 25:RA:2867:G:HO2'  | 25:RA:2868:A:H8     | 1.34                     | 0.75              |
| 41:RV:15:GLU:O     | 41:RV:18:LEU:HB2    | 1.86                     | 0.75              |
| 41:RV:47:VAL:HG13  | 41:RV:48:GLY:H      | 1.49                     | 0.75              |
| 44:RY:48:ALA:O     | 44:RY:49:VAL:C      | 2.30                     | 0.75              |
| 1:XA:448:A:OP2     | 1:XA:485:G:N2       | 2.17                     | 0.75              |
| 7:XG:148:ASN:HD22  | 7:XG:148:ASN:N      | 1.82                     | 0.75              |
| 25:YA:676:A:H8     | 25:YA:2069:G:H21    | 1.33                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:2452:C:O4'  | 56:Z8:76:PPU:HB2  | 1.85                     | 0.75              |
| 8:QH:1:MET:HE2    | 8:QH:1:MET:H3     | 1.49                     | 0.75              |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:HA   | 1.67                     | 0.75              |
| 44:RY:90:LEU:N    | 44:RY:90:LEU:HD22 | 2.02                     | 0.75              |
| 47:R1:80:LEU:C    | 47:R1:81:LYS:HE2  | 2.10                     | 0.75              |
| 1:XA:411:A:H62    | 1:XA:413:G:H21    | 1.35                     | 0.75              |
| 4:XD:153:ARG:NH1  | 4:XD:181:MET:HG3  | 2.00                     | 0.75              |
| 41:YV:35:LEU:H    | 41:YV:35:LEU:HD22 | 1.51                     | 0.75              |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:CB   | 1.98                     | 0.75              |
| 47:Y1:80:LEU:C    | 47:Y1:81:LYS:HD2  | 2.12                     | 0.75              |
| 1:QA:1054:C:OP2   | 1:QA:1197:G:OP2   | 2.05                     | 0.75              |
| 4:QD:26:CYS:HA    | 4:QD:31:CYS:HB2   | 1.67                     | 0.75              |
| 11:QK:77:MET:HE3  | 11:QK:80:VAL:HG12 | 1.67                     | 0.75              |
| 19:QS:39:THR:HG22 | 19:QS:40:ILE:H    | 1.50                     | 0.75              |
| 19:QS:41:VAL:HG12 | 19:QS:44:MET:H    | 1.50                     | 0.75              |
| 25:RA:637:A:H2'   | 35:RP:117:GLU:OE2 | 1.87                     | 0.75              |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:H   | 1.52                     | 0.75              |
| 47:R1:3:LYS:HD3   | 47:R1:43:TYR:HD2  | 1.52                     | 0.75              |
| 7:XG:23:VAL:HG12  | 7:XG:27:ILE:HD11  | 1.69                     | 0.75              |
| 20:XT:26:ASN:O    | 20:XT:30:LYS:HB2  | 1.85                     | 0.75              |
| 20:XT:58:LYS:HE3  | 20:XT:62:LEU:HD11 | 1.69                     | 0.75              |
| 33:YN:42:TRP:HA   | 33:YN:48:MET:HE1  | 1.69                     | 0.75              |
| 35:YP:75:ILE:HD13 | 35:YP:75:ILE:N    | 2.00                     | 0.75              |
| 37:YR:33:ARG:HH22 | 51:Y5:55:ARG:HG2  | 1.51                     | 0.75              |
| 39:YT:43:GLN:HG2  | 39:YT:44:ASP:N    | 1.99                     | 0.75              |
| 41:YV:51:VAL:HG12 | 41:YV:52:VAL:H    | 1.52                     | 0.75              |
| 42:YW:40:ASN:O    | 42:YW:41:LYS:HG2  | 1.86                     | 0.75              |
| 6:QF:60:PHE:C     | 6:QF:61:LEU:HD12  | 2.12                     | 0.75              |
| 20:QT:35:THR:O    | 20:QT:39:LYS:HG3  | 1.87                     | 0.75              |
| 25:RA:2115:G:N2   | 25:RA:2165:G:N7   | 2.31                     | 0.75              |
| 28:RE:63:LEU:CD1  | 28:RE:65:GLY:H    | 1.99                     | 0.75              |
| 30:RG:97:ASP:H    | 30:RG:100:TRP:HD1 | 1.31                     | 0.75              |
| 37:RR:73:VAL:O    | 37:RR:76:VAL:HG12 | 1.87                     | 0.75              |
| 8:XH:91:ARG:HH11  | 8:XH:91:ARG:HG2   | 1.51                     | 0.75              |
| 19:XS:41:VAL:HG12 | 19:XS:44:MET:H    | 1.50                     | 0.75              |
| 27:YD:146:GLU:HB2 | 27:YD:189:CYS:HB3 | 1.67                     | 0.75              |
| 29:YF:7:TYR:HB3   | 29:YF:21:ALA:CB   | 2.16                     | 0.75              |
| 37:YR:73:VAL:O    | 37:YR:76:VAL:HG12 | 1.87                     | 0.75              |
| 44:YY:90:LEU:HD22 | 44:YY:90:LEU:N    | 2.02                     | 0.75              |
| 47:Y1:80:LEU:O    | 47:Y1:81:LYS:CB   | 2.35                     | 0.75              |
| 13:QM:3:ARG:CA    | 13:QM:9:ILE:HG21  | 2.13                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:RE:36:ARG:HH21  | 28:RE:88:GLY:HA2  | 1.51                     | 0.74              |
| 34:RO:107:ARG:HA   | 34:RO:112:MET:HE1 | 1.67                     | 0.74              |
| 38:RS:62:LYS:HB3   | 38:RS:97:ARG:HD3  | 1.69                     | 0.74              |
| 42:RW:40:ASN:O     | 42:RW:41:LYS:HG2  | 1.86                     | 0.74              |
| 15:XO:74:ASP:CG    | 15:XO:77:ARG:HG2  | 2.12                     | 0.74              |
| 21:XU:10:ARG:HG2   | 21:XU:13:ILE:HD12 | 1.68                     | 0.74              |
| 25:YA:1728:G:N1    | 25:YA:1730:U:OP2  | 2.21                     | 0.74              |
| 44:YY:97:ARG:NH2   | 44:YY:98:VAL:HB   | 2.01                     | 0.74              |
| 51:Y5:47:PRO:O     | 51:Y5:48:GLU:HG3  | 1.86                     | 0.74              |
| 13:QM:37:THR:HG21  | 13:QM:39:ILE:HD11 | 1.68                     | 0.74              |
| 16:QP:43:LYS:HG2   | 16:QP:48:TRP:CE3  | 2.22                     | 0.74              |
| 33:RN:96:GLU:CG    | 33:RN:97:ARG:H    | 2.00                     | 0.74              |
| 40:RU:92:ARG:HH11  | 40:RU:95:LEU:CD1  | 2.00                     | 0.74              |
| 42:RW:18:ARG:HG3   | 42:RW:76:VAL:CG1  | 2.15                     | 0.74              |
| 48:R2:41:ILE:C     | 48:R2:41:ILE:HD12 | 2.10                     | 0.74              |
| 7:XG:9:VAL:HG13    | 7:XG:94:ARG:HE    | 1.53                     | 0.74              |
| 24:XX:2:U:C2'      | 24:XX:3:G:H5'     | 2.17                     | 0.74              |
| 15:QO:70:LEU:HD12  | 15:QO:70:LEU:O    | 1.88                     | 0.74              |
| 15:QO:87:ILE:HG22  | 15:QO:88:ARG:N    | 2.00                     | 0.74              |
| 24:QX:2:U:C2'      | 24:QX:3:G:H5'     | 2.17                     | 0.74              |
| 25:RA:2701:C:H3'   | 25:RA:2702:U:C5'  | 2.16                     | 0.74              |
| 39:RT:111:ARG:O    | 39:RT:113:LYS:N   | 2.17                     | 0.74              |
| 43:RX:57:LEU:HD11  | 43:RX:78:LYS:HB2  | 1.68                     | 0.74              |
| 47:R1:26:ARG:O     | 47:R1:26:ARG:HD2  | 1.86                     | 0.74              |
| 2:XB:101:MET:CA    | 2:XB:108:ILE:HG13 | 2.11                     | 0.74              |
| 5:XE:10:MET:CB     | 5:XE:32:VAL:HG22  | 2.18                     | 0.74              |
| 5:XE:72:GLN:NE2    | 5:XE:144:THR:HG22 | 2.01                     | 0.74              |
| 19:XS:3:ARG:HG3    | 19:XS:4:SER:H     | 1.52                     | 0.74              |
| 25:YA:1113:U:OP1   | 31:YH:2:SER:N     | 2.20                     | 0.74              |
| 28:YE:61:ARG:HB2   | 28:YE:62:PRO:HD3  | 1.69                     | 0.74              |
| 35:YP:64:LYS:C     | 35:YP:66:GLY:H    | 1.94                     | 0.74              |
| 39:YT:78:LEU:HD13  | 39:YT:78:LEU:O    | 1.87                     | 0.74              |
| 40:YU:52:ARG:HH11  | 40:YU:52:ARG:HG2  | 1.51                     | 0.74              |
| 44:YY:51:VAL:HG13  | 44:YY:52:SER:N    | 2.02                     | 0.74              |
| 49:Y3:7:LYS:HB2    | 49:Y3:34:GLU:HG2  | 1.69                     | 0.74              |
| 9:QI:62:TYR:C      | 9:QI:63:ILE:HD12  | 2.12                     | 0.74              |
| 9:QI:113:LYS:HD2   | 9:QI:113:LYS:H    | 1.51                     | 0.74              |
| 29:RF:136:THR:HG22 | 29:RF:166:ALA:O   | 1.87                     | 0.74              |
| 41:RV:52:VAL:HG21  | 41:RV:55:ALA:HB3  | 1.68                     | 0.74              |
| 11:XK:48:ILE:HD11  | 11:XK:64:ALA:HA   | 1.68                     | 0.74              |
| 27:YD:54:ARG:HG3   | 27:YD:54:ARG:HH11 | 1.49                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:26:ASP:HB3   | 39:YT:91:ARG:HA    | 1.69                     | 0.74              |
| 47:Y1:26:ARG:O     | 47:Y1:26:ARG:HD2   | 1.86                     | 0.74              |
| 15:QO:74:ASP:CG    | 15:QO:77:ARG:HG2   | 2.12                     | 0.74              |
| 29:RF:7:TYR:HB3    | 29:RF:21:ALA:CB    | 2.16                     | 0.74              |
| 34:RO:26:LYS:HB2   | 34:RO:30:ALA:CB    | 2.18                     | 0.74              |
| 35:RP:64:LYS:C     | 35:RP:66:GLY:H     | 1.94                     | 0.74              |
| 9:XI:128:ARG:HH21  | 22:XV:35:A:P       | 2.09                     | 0.74              |
| 16:XP:43:LYS:O     | 16:XP:45:THR:N     | 2.21                     | 0.74              |
| 27:YD:30:GLU:HG3   | 27:YD:63:ARG:CZ    | 2.18                     | 0.74              |
| 36:YQ:79:LEU:O     | 36:YQ:79:LEU:CD2   | 2.36                     | 0.74              |
| 4:QD:166:LYS:HD3   | 27:YD:134:ARG:NH1  | 2.03                     | 0.74              |
| 10:QJ:33:GLN:O     | 10:QJ:75:ILE:HG12  | 1.87                     | 0.74              |
| 48:R2:47:ASN:HD22  | 48:R2:47:ASN:H     | 1.33                     | 0.74              |
| 2:XB:178:ARG:NH2   | 8:XH:74:PRO:HB3    | 2.02                     | 0.74              |
| 4:XD:25:ARG:HH12   | 4:XD:30:LYS:HG3    | 1.52                     | 0.74              |
| 6:XF:60:PHE:C      | 6:XF:61:LEU:HD12   | 2.12                     | 0.74              |
| 7:XG:78:ARG:HH12   | 7:XG:80:VAL:HG23   | 1.52                     | 0.74              |
| 10:XJ:33:GLN:O     | 10:XJ:75:ILE:HG12  | 1.87                     | 0.74              |
| 17:XQ:59:ILE:H     | 17:XQ:59:ILE:HD13  | 1.50                     | 0.74              |
| 20:XT:35:THR:O     | 20:XT:39:LYS:HG3   | 1.87                     | 0.74              |
| 25:YA:2680:C:H5'   | 28:YE:189:PRO:HA   | 1.67                     | 0.74              |
| 33:YN:96:GLU:HG2   | 33:YN:97:ARG:N     | 2.01                     | 0.74              |
| 49:Y3:29:ARG:HB2   | 49:Y3:29:ARG:HH11  | 1.52                     | 0.74              |
| 1:QA:1318:A:H4'    | 19:QS:11:VAL:HG11  | 1.69                     | 0.74              |
| 2:QB:168:THR:HB    | 2:QB:192:SER:HB2   | 1.70                     | 0.74              |
| 25:RA:579:G:O2'    | 25:RA:2019:A:OP1   | 2.06                     | 0.74              |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:HB3  | 1.70                     | 0.74              |
| 38:RS:83:LYS:HZ2   | 38:RS:109:GLY:HA2  | 1.49                     | 0.74              |
| 44:RY:44:ILE:HG13  | 44:RY:45:VAL:N     | 2.00                     | 0.74              |
| 49:R3:29:ARG:HH11  | 49:R3:29:ARG:HB2   | 1.52                     | 0.74              |
| 50:R4:71:ARG:HG3   | 50:R4:71:ARG:NH1   | 1.90                     | 0.74              |
| 31:YH:150:ALA:C    | 31:YH:152:ARG:N    | 2.44                     | 0.74              |
| 31:YH:153:LYS:HG2  | 31:YH:162:ILE:H    | 1.52                     | 0.74              |
| 39:YT:54:ARG:HG2   | 39:YT:54:ARG:HH11  | 1.52                     | 0.74              |
| 40:YU:64:ARG:HH21  | 40:YU:64:ARG:CG    | 2.00                     | 0.74              |
| 7:QG:9:VAL:HG13    | 7:QG:94:ARG:HE     | 1.53                     | 0.74              |
| 25:RA:1190:G:OP1   | 35:RP:30:THR:OG1   | 2.03                     | 0.74              |
| 27:RD:77:ALA:CB    | 27:RD:97:TYR:HA    | 2.18                     | 0.74              |
| 39:RT:50:ILE:HD12  | 39:RT:102:ILE:HD11 | 1.68                     | 0.74              |
| 41:RV:1:MET:HE2    | 41:RV:43:GLU:CG    | 2.17                     | 0.74              |
| 1:XA:28:G:O2'      | 1:XA:296:U:OP1     | 2.04                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:236:G:OP1     | 17:XQ:40:LYS:NZ    | 2.21                     | 0.74              |
| 1:XA:951:G:OP2     | 13:XM:102:ARG:NH2  | 2.21                     | 0.74              |
| 3:XC:181:ASN:ND2   | 3:XC:204:LEU:HD12  | 1.99                     | 0.74              |
| 6:XF:91:VAL:HG13   | 18:XR:72:ARG:HH12  | 1.51                     | 0.74              |
| 29:YF:129:PHE:HA   | 29:YF:142:TRP:NE1  | 2.02                     | 0.74              |
| 38:YS:36:TYR:CD2   | 38:YS:52:SER:HB3   | 2.23                     | 0.74              |
| 41:YV:15:GLU:O     | 41:YV:18:LEU:HB2   | 1.86                     | 0.74              |
| 4:QD:91:SER:HA     | 4:QD:94:LEU:HD13   | 1.70                     | 0.74              |
| 6:QF:19:LEU:HD23   | 6:QF:19:LEU:O      | 1.88                     | 0.74              |
| 26:RB:55:U:C4'     | 30:RG:29:TRP:HE1   | 2.01                     | 0.74              |
| 41:RV:35:LEU:H     | 41:RV:35:LEU:HD22  | 1.51                     | 0.74              |
| 44:RY:95:LYS:HB3   | 44:RY:100:ALA:CA   | 2.10                     | 0.74              |
| 6:XF:19:LEU:O      | 6:XF:19:LEU:HD23   | 1.88                     | 0.74              |
| 13:XM:37:THR:HG21  | 13:XM:39:ILE:HD11  | 1.68                     | 0.74              |
| 15:XO:70:LEU:HD12  | 15:XO:70:LEU:O     | 1.88                     | 0.74              |
| 29:YF:136:THR:HG22 | 29:YF:166:ALA:O    | 1.87                     | 0.74              |
| 1:QA:606:G:H22     | 1:QA:631:G:H5'     | 1.53                     | 0.74              |
| 2:QB:47:THR:O      | 2:QB:51:LEU:HG     | 1.87                     | 0.74              |
| 5:QE:72:GLN:HE21   | 5:QE:144:THR:HG22  | 1.53                     | 0.74              |
| 7:QG:23:VAL:HG12   | 7:QG:27:ILE:HD11   | 1.69                     | 0.74              |
| 13:QM:77:ASN:HA    | 50:R4:71:ARG:HH22  | 1.52                     | 0.74              |
| 25:RA:1021:A:OP2   | 33:RN:65:LYS:NZ    | 2.20                     | 0.74              |
| 34:RO:47:ILE:CD1   | 34:RO:48:PRO:HD2   | 2.16                     | 0.74              |
| 35:RP:19:VAL:HG22  | 35:RP:20:GLY:N     | 1.97                     | 0.74              |
| 35:RP:62:LEU:HD22  | 35:RP:62:LEU:H     | 1.53                     | 0.74              |
| 42:RW:70:TYR:HD2   | 42:RW:70:TYR:H     | 1.36                     | 0.74              |
| 42:RW:73:ALA:HB3   | 42:RW:106:ILE:HG12 | 1.68                     | 0.74              |
| 44:RY:52:SER:OG    | 44:RY:53:PRO:HD3   | 1.88                     | 0.74              |
| 47:R1:80:LEU:O     | 47:R1:81:LYS:CB    | 2.35                     | 0.74              |
| 10:XJ:27:ALA:HB1   | 10:XJ:34:VAL:HG21  | 1.69                     | 0.74              |
| 25:YA:1479:G:N7    | 25:YA:1510:A:N6    | 2.35                     | 0.74              |
| 29:YF:29:ASN:HB3   | 29:YF:112:MET:HE1  | 1.70                     | 0.74              |
| 33:YN:56:ASN:HD22  | 33:YN:125:GLY:C    | 1.96                     | 0.74              |
| 41:YV:1:MET:HE2    | 41:YV:43:GLU:CG    | 2.17                     | 0.74              |
| 2:QB:115:LEU:HD13  | 2:QB:145:LEU:HB3   | 1.68                     | 0.73              |
| 3:QC:86:VAL:O      | 3:QC:89:GLU:HB3    | 1.88                     | 0.73              |
| 10:QJ:3:LYS:HD2    | 10:QJ:77:PRO:HD3   | 1.70                     | 0.73              |
| 33:RN:58:ASP:H     | 33:RN:60:ILE:HD11  | 1.53                     | 0.73              |
| 35:RP:50:ARG:HB3   | 35:RP:50:ARG:NH2   | 1.98                     | 0.73              |
| 36:RQ:79:LEU:O     | 36:RQ:79:LEU:CD1   | 2.35                     | 0.73              |
| 38:RS:36:TYR:CD2   | 38:RS:52:SER:HB3   | 2.23                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:RV:51:VAL:HG12 | 41:RV:52:VAL:H     | 1.52                     | 0.73              |
| 47:R1:76:ARG:HH11 | 47:R1:76:ARG:HG2   | 1.53                     | 0.73              |
| 51:R5:2:ALA:O     | 51:R5:3:LYS:HB2    | 1.88                     | 0.73              |
| 5:XE:45:PHE:CE2   | 5:XE:47:LYS:HD2    | 2.22                     | 0.73              |
| 5:XE:72:GLN:HE21  | 5:XE:144:THR:HG22  | 1.53                     | 0.73              |
| 27:YD:131:LEU:HB2 | 27:YD:136:ILE:CD1  | 2.17                     | 0.73              |
| 50:Y4:41:PRO:O    | 50:Y4:42:PHE:HB3   | 1.87                     | 0.73              |
| 13:QM:119:GLY:HA3 | 22:QV:29:G:OP1     | 1.88                     | 0.73              |
| 14:QN:40:CYS:SG   | 14:QN:42:ILE:HB    | 2.27                     | 0.73              |
| 28:RE:61:ARG:HB2  | 28:RE:62:PRO:HD3   | 1.69                     | 0.73              |
| 3:XC:134:ILE:HD11 | 3:XC:153:VAL:HG21  | 1.70                     | 0.73              |
| 14:YN:44:LEU:CD1  | 14:YN:53:LEU:CD1   | 2.66                     | 0.73              |
| 19:XS:68:GLY:HA3  | 50:Y4:68:ARG:HB2   | 1.70                     | 0.73              |
| 25:YA:155:C:N4    | 25:YA:171:G:O6     | 2.19                     | 0.73              |
| 28:YE:78:LEU:HG   | 28:YE:79:ARG:NE    | 2.03                     | 0.73              |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:H     | 1.52                     | 0.73              |
| 29:RF:29:ASN:HB3  | 29:RF:112:MET:HE1  | 1.70                     | 0.73              |
| 2:XB:47:THR:O     | 2:XB:51:LEU:HG     | 1.87                     | 0.73              |
| 25:YA:1077:A:H5'  | 25:YA:1078:U:H5''  | 1.70                     | 0.73              |
| 34:YO:26:LYS:HB2  | 34:YO:30:ALA:CB    | 2.18                     | 0.73              |
| 1:QA:1269:A:N1    | 1:QA:1312:G:O2'    | 2.21                     | 0.73              |
| 3:QC:134:ILE:HD11 | 3:QC:153:VAL:HG21  | 1.70                     | 0.73              |
| 25:RA:2131:G:H4'  | 25:RA:2132:U:H4'   | 1.70                     | 0.73              |
| 29:RF:9:ILE:HD11  | 29:RF:125:LEU:HG   | 1.70                     | 0.73              |
| 39:RT:23:ARG:HB2  | 39:RT:24:PRO:HD2   | 1.70                     | 0.73              |
| 2:XB:8:LYS:HD3    | 2:XB:8:LYS:N       | 2.03                     | 0.73              |
| 14:YN:32:SER:O    | 14:YN:41:ARG:N     | 2.22                     | 0.73              |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:CA   | 2.18                     | 0.73              |
| 39:YT:102:ILE:HB  | 39:YT:110:ILE:CD1  | 2.19                     | 0.73              |
| 27:RD:30:GLU:HG3  | 27:RD:63:ARG:CZ    | 2.17                     | 0.73              |
| 47:R1:80:LEU:C    | 47:R1:81:LYS:HD2   | 2.12                     | 0.73              |
| 1:QA:191:G:C4     | 20:QT:105:SER:HB3  | 2.24                     | 0.73              |
| 16:QP:43:LYS:O    | 16:QP:45:THR:N     | 2.21                     | 0.73              |
| 25:RA:768:G:O2'   | 25:RA:1379:A:N6    | 2.22                     | 0.73              |
| 28:RE:23:VAL:HG21 | 28:RE:183:LEU:HD23 | 1.68                     | 0.73              |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:CA   | 2.18                     | 0.73              |
| 33:RN:96:GLU:HG2  | 33:RN:97:ARG:N     | 2.01                     | 0.73              |
| 40:RU:64:ARG:HH21 | 40:RU:64:ARG:CG    | 2.00                     | 0.73              |
| 3:XC:107:GLN:CD   | 3:XC:107:GLN:H     | 1.97                     | 0.73              |
| 16:XP:60:LEU:HA   | 16:XP:64:ALA:HB3   | 1.71                     | 0.73              |
| 44:YY:48:ALA:O    | 44:YY:49:VAL:C     | 2.30                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:Y4:29:PRO:O    | 50:Y4:30:GLU:HB2   | 1.89                     | 0.73              |
| 1:QA:235:C:H5'    | 17:QQ:70:ARG:HG2   | 1.69                     | 0.73              |
| 5:QE:10:MET:CB    | 5:QE:32:VAL:HG22   | 2.17                     | 0.73              |
| 7:QG:79:ARG:HH22  | 7:QG:82:GLY:HA2    | 1.51                     | 0.73              |
| 25:RA:2781:A:H5'' | 25:RA:2782:G:H5'   | 1.70                     | 0.73              |
| 27:RD:131:LEU:HB2 | 27:RD:136:ILE:CD1  | 2.17                     | 0.73              |
| 28:RE:203:LYS:O   | 28:RE:203:LYS:HD2  | 1.89                     | 0.73              |
| 31:RH:84:SER:O    | 31:RH:85:LYS:HB2   | 1.89                     | 0.73              |
| 31:RH:125:VAL:HA  | 31:RH:126:PRO:HB3  | 1.68                     | 0.73              |
| 50:R4:41:PRO:O    | 50:R4:42:PHE:HB3   | 1.88                     | 0.73              |
| 3:XC:86:VAL:O     | 3:XC:89:GLU:HB3    | 1.88                     | 0.73              |
| 18:XR:56:THR:HB   | 18:XR:58:LEU:HD12  | 1.71                     | 0.73              |
| 25:YA:1403:C:H5'' | 25:YA:1471:A:H1'   | 1.71                     | 0.73              |
| 28:YE:203:LYS:O   | 28:YE:203:LYS:HD2  | 1.88                     | 0.73              |
| 38:YS:62:LYS:HB3  | 38:YS:97:ARG:HD3   | 1.68                     | 0.73              |
| 48:Y2:29:LYS:HD3  | 48:Y2:57:ILE:HD13  | 1.71                     | 0.73              |
| 51:Y5:40:LYS:CE   | 51:Y5:46:CYS:HB3   | 2.19                     | 0.73              |
| 2:QB:132:LYS:HA   | 2:QB:135:GLN:HB2   | 1.71                     | 0.73              |
| 4:QD:30:LYS:HB2   | 4:QD:35:ARG:HG3    | 1.70                     | 0.73              |
| 29:RF:157:VAL:HB  | 29:RF:194:MET:HB3  | 1.70                     | 0.73              |
| 39:RT:26:ASP:HB3  | 39:RT:91:ARG:HA    | 1.69                     | 0.73              |
| 40:RU:34:LYS:HE2  | 40:RU:34:LYS:HA    | 1.70                     | 0.73              |
| 49:R3:7:LYS:HB2   | 49:R3:34:GLU:HG2   | 1.70                     | 0.73              |
| 4:XD:146:ILE:HD12 | 4:XD:146:ILE:N     | 2.04                     | 0.73              |
| 8:XH:20:TYR:HD1   | 8:XH:65:TYR:CD2    | 2.07                     | 0.73              |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:H     | 1.52                     | 0.73              |
| 54:Y8:61:LEU:O    | 54:Y8:62:LEU:HB2   | 1.88                     | 0.73              |
| 1:QA:677:U:H3     | 1:QA:713:G:H22     | 1.34                     | 0.73              |
| 16:QP:3:LYS:C     | 16:QP:4:ILE:HD12   | 2.14                     | 0.73              |
| 20:QT:50:GLU:HG3  | 20:QT:51:GLU:H     | 1.54                     | 0.73              |
| 25:RA:1803:A:H4'  | 27:RD:259:THR:HG21 | 1.70                     | 0.73              |
| 35:RP:15:ARG:O    | 35:RP:16:ARG:C     | 2.32                     | 0.73              |
| 2:XB:115:LEU:HD13 | 2:XB:145:LEU:HB3   | 1.69                     | 0.73              |
| 7:XG:8:GLU:CD     | 7:XG:8:GLU:H       | 1.96                     | 0.73              |
| 29:YF:29:ASN:H    | 29:YF:112:MET:HE1  | 1.54                     | 0.73              |
| 36:YQ:79:LEU:O    | 36:YQ:79:LEU:CD1   | 2.35                     | 0.73              |
| 11:QK:48:ILE:HD12 | 11:QK:63:LEU:HB3   | 1.71                     | 0.73              |
| 13:QM:121:LYS:HE2 | 13:QM:121:LYS:HA   | 1.71                     | 0.73              |
| 19:QS:3:ARG:HG3   | 19:QS:4:SER:H      | 1.52                     | 0.73              |
| 31:RH:80:SER:O    | 31:RH:81:GLU:HB2   | 1.89                     | 0.73              |
| 33:RN:42:TRP:HA   | 33:RN:48:MET:HE1   | 1.69                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:90:VAL:CG1   | 36:RQ:91:GLU:H     | 2.02                     | 0.73              |
| 48:R2:27:GLU:OE1   | 48:R2:27:GLU:N     | 2.19                     | 0.73              |
| 3:XC:13:GLY:HA3    | 14:XN:57:ARG:NH2   | 2.04                     | 0.73              |
| 6:XF:77:ARG:HB2    | 6:XF:77:ARG:HH11   | 1.53                     | 0.73              |
| 12:XL:48:PRO:HD2   | 12:XL:49:ASN:H     | 1.51                     | 0.73              |
| 19:XS:5:LEU:CD1    | 50:Y4:66:SER:HB2   | 2.16                     | 0.73              |
| 20:XT:47:GLY:O     | 20:XT:49:ALA:N     | 2.19                     | 0.73              |
| 27:YD:77:ALA:CB    | 27:YD:97:TYR:HA    | 2.18                     | 0.73              |
| 30:YG:7:LEU:HD21   | 30:YG:176:LEU:HD22 | 1.70                     | 0.73              |
| 31:YH:153:LYS:HA   | 31:YH:153:LYS:HZ3  | 1.52                     | 0.73              |
| 33:YN:58:ASP:H     | 33:YN:60:ILE:HD11  | 1.53                     | 0.73              |
| 37:YR:3:HIS:O      | 37:YR:5:LYS:N      | 2.22                     | 0.73              |
| 54:Y8:16:ILE:HD11  | 54:Y8:57:ARG:HG2   | 1.69                     | 0.73              |
| 3:QC:107:GLN:CD    | 3:QC:107:GLN:H     | 1.97                     | 0.72              |
| 6:QF:25:ILE:HD13   | 6:QF:28:ARG:NH1    | 2.04                     | 0.72              |
| 16:QP:45:THR:HG23  | 16:QP:46:PRO:HD2   | 1.71                     | 0.72              |
| 29:RF:101:LEU:CD1  | 29:RF:102:PRO:HD2  | 2.11                     | 0.72              |
| 31:RH:54:ARG:HH12  | 31:RH:62:LYS:HG2   | 1.54                     | 0.72              |
| 1:XA:328:C:H4'     | 1:XA:329:A:H5'     | 1.71                     | 0.72              |
| 1:XA:1112:C:H1'    | 3:XC:179:ARG:HH11  | 1.54                     | 0.72              |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:HG3  | 1.71                     | 0.72              |
| 35:YP:126:VAL:CG1  | 35:YP:147:LEU:HD21 | 2.17                     | 0.72              |
| 4:QD:30:LYS:HG3    | 4:QD:35:ARG:HE     | 1.52                     | 0.72              |
| 25:RA:704:G:H2'    | 25:RA:726:G:H22    | 1.53                     | 0.72              |
| 28:RE:13:ARG:HA    | 28:RE:22:PRO:HA    | 1.71                     | 0.72              |
| 28:RE:56:PRO:O     | 28:RE:57:LYS:HB2   | 1.89                     | 0.72              |
| 1:XA:1321:C:H5''   | 1:XA:1322:C:H5''   | 1.70                     | 0.72              |
| 2:XB:75:LYS:O      | 2:XB:75:LYS:HD3    | 1.89                     | 0.72              |
| 4:XD:91:SER:HA     | 4:XD:94:LEU:HD13   | 1.70                     | 0.72              |
| 33:YN:89:LYS:O     | 33:YN:93:THR:HG22  | 1.89                     | 0.72              |
| 44:YY:52:SER:OG    | 44:YY:53:PRO:HD3   | 1.88                     | 0.72              |
| 49:Y3:56:VAL:HG12  | 49:Y3:57:GLU:N     | 2.04                     | 0.72              |
| 51:Y5:58:LEU:CD1   | 51:Y5:60:VAL:HG12  | 2.18                     | 0.72              |
| 1:QA:375:U:H4'     | 16:QP:17:TYR:HE2   | 1.51                     | 0.72              |
| 1:QA:489:C:OP1     | 4:QD:132:ARG:NH2   | 2.21                     | 0.72              |
| 1:QA:1330:U:OP1    | 13:QM:25:ILE:O     | 2.06                     | 0.72              |
| 30:RG:146:TYR:O    | 30:RG:149:VAL:HG22 | 1.88                     | 0.72              |
| 13:XM:93:ARG:NH1   | 25:YA:887:A:OP1    | 2.22                     | 0.72              |
| 16:XP:20:VAL:HG21  | 16:XP:32:TYR:CG    | 2.24                     | 0.72              |
| 31:YH:152:ARG:O    | 31:YH:153:LYS:HD2  | 1.90                     | 0.72              |
| 36:YQ:90:VAL:CG1   | 36:YQ:91:GLU:H     | 2.02                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:YR:117:VAL:HG22 | 37:YR:118:GLU:N    | 2.05                     | 0.72              |
| 38:YS:83:LYS:HZ2   | 38:YS:109:GLY:HA2  | 1.54                     | 0.72              |
| 40:YU:98:LEU:HD23  | 40:YU:99:ALA:N     | 2.04                     | 0.72              |
| 52:Y6:13:CYS:HA    | 52:Y6:50:ARG:O     | 1.90                     | 0.72              |
| 5:QE:36:ASP:OD2    | 5:QE:38:GLN:HB2    | 1.86                     | 0.72              |
| 15:QO:71:GLN:HB2   | 15:QO:78:TYR:CD1   | 2.25                     | 0.72              |
| 25:RA:2745:C:O2    | 31:RH:139:GLN:NE2  | 2.22                     | 0.72              |
| 26:RB:55:U:H4'     | 30:RG:29:TRP:NE1   | 2.02                     | 0.72              |
| 39:RT:117:ASP:O    | 39:RT:121:ILE:HG13 | 1.89                     | 0.72              |
| 42:RW:1:MET:HA     | 42:RW:1:MET:HE3    | 1.71                     | 0.72              |
| 51:R5:40:LYS:CE    | 51:R5:46:CYS:HB3   | 2.19                     | 0.72              |
| 19:XS:5:LEU:HD22   | 50:Y4:67:TYR:CZ    | 2.23                     | 0.72              |
| 30:YG:146:TYR:O    | 30:YG:149:VAL:HG22 | 1.89                     | 0.72              |
| 35:YP:15:ARG:O     | 35:YP:16:ARG:C     | 2.32                     | 0.72              |
| 41:YV:39:LEU:O     | 41:YV:40:LEU:HD23  | 1.90                     | 0.72              |
| 47:Y1:80:LEU:HB2   | 47:Y1:81:LYS:HE2   | 1.71                     | 0.72              |
| 54:Y8:29:LYS:HD3   | 54:Y8:44:LYS:HB2   | 1.71                     | 0.72              |
| 1:QA:1106:G:H5''   | 3:QC:172:ARG:HG2   | 1.72                     | 0.72              |
| 3:QC:13:GLY:HA3    | 14:QN:57:ARG:NH2   | 2.04                     | 0.72              |
| 7:QG:78:ARG:HH12   | 7:QG:80:VAL:HG23   | 1.53                     | 0.72              |
| 15:QO:79:ARG:O     | 15:QO:82:ILE:HG22  | 1.89                     | 0.72              |
| 28:RE:78:LEU:HG    | 28:RE:79:ARG:NE    | 2.03                     | 0.72              |
| 31:RH:30:LYS:HD2   | 31:RH:81:GLU:H     | 1.54                     | 0.72              |
| 34:RO:113:LYS:HG2  | 34:RO:117:LEU:HD11 | 1.71                     | 0.72              |
| 38:RS:42:ASP:O     | 38:RS:43:GLU:HB2   | 1.90                     | 0.72              |
| 54:R8:59:LYS:CB    | 54:R8:59:LYS:HZ3   | 2.01                     | 0.72              |
| 3:XC:16:ARG:HB2    | 3:XC:16:ARG:NH1    | 2.04                     | 0.72              |
| 8:XH:41:ARG:HH11   | 8:XH:41:ARG:CB     | 2.03                     | 0.72              |
| 29:YF:124:LEU:HD12 | 29:YF:125:LEU:N    | 2.04                     | 0.72              |
| 31:YH:54:ARG:HH12  | 31:YH:62:LYS:HG2   | 1.54                     | 0.72              |
| 36:YQ:81:VAL:HG23  | 46:Y0:7:LEU:HD21   | 1.71                     | 0.72              |
| 37:YR:85:PRO:O     | 37:YR:87:TYR:N     | 2.22                     | 0.72              |
| 48:Y2:27:GLU:OE1   | 48:Y2:27:GLU:N     | 2.19                     | 0.72              |
| 4:QD:146:ILE:HD12  | 4:QD:146:ILE:N     | 2.04                     | 0.72              |
| 12:QL:126:LYS:HB2  | 12:QL:126:LYS:NZ   | 2.04                     | 0.72              |
| 39:RT:54:ARG:HH11  | 39:RT:54:ARG:HG2   | 1.52                     | 0.72              |
| 39:RT:78:LEU:HD13  | 39:RT:78:LEU:O     | 1.87                     | 0.72              |
| 47:R1:80:LEU:HB2   | 47:R1:81:LYS:HE2   | 1.71                     | 0.72              |
| 54:R8:16:ILE:HD11  | 54:R8:57:ARG:HG2   | 1.69                     | 0.72              |
| 1:XA:1152:A:H5''   | 10:XJ:13:HIS:CD2   | 2.25                     | 0.72              |
| 2:XB:21:ARG:O      | 2:XB:23:ARG:HD3    | 1.89                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:14:ILE:HD11  | 39:YT:14:TYR:OH    | 1.90                     | 0.72              |
| 28:YE:21:VAL:HB    | 28:YE:22:PRO:CB    | 2.18                     | 0.72              |
| 31:YH:132:ARG:HH11 | 31:YH:132:ARG:CB   | 1.97                     | 0.72              |
| 38:YS:26:LEU:O     | 38:YS:26:LEU:HD23  | 1.90                     | 0.72              |
| 40:YU:34:LYS:HE2   | 40:YU:34:LYS:HA    | 1.69                     | 0.72              |
| 6:QF:72:VAL:CG2    | 6:QF:90:VAL:HG11   | 2.20                     | 0.72              |
| 20:QT:27:LYS:O     | 20:QT:30:LYS:HB3   | 1.89                     | 0.72              |
| 20:QT:97:ALA:O     | 20:QT:99:LEU:HD13  | 1.89                     | 0.72              |
| 28:RE:28:ALA:HB3   | 28:RE:93:VAL:HG22  | 1.72                     | 0.72              |
| 29:RF:124:LEU:HD12 | 29:RF:125:LEU:N    | 2.04                     | 0.72              |
| 31:RH:26:VAL:CG1   | 31:RH:27:LYS:H     | 2.02                     | 0.72              |
| 33:RN:56:ASN:HD22  | 33:RN:125:GLY:C    | 1.96                     | 0.72              |
| 38:RS:103:GLU:O    | 38:RS:106:ARG:HG3  | 1.90                     | 0.72              |
| 45:RZ:150:LEU:HD21 | 45:RZ:172:ALA:HB3  | 1.71                     | 0.72              |
| 49:R3:56:VAL:HG12  | 49:R3:57:GLU:N     | 2.04                     | 0.72              |
| 51:R5:58:LEU:CD1   | 51:R5:60:VAL:HG12  | 2.19                     | 0.72              |
| 10:XJ:3:LYS:HD2    | 10:XJ:77:PRO:HD3   | 1.70                     | 0.72              |
| 16:XP:3:LYS:C      | 16:XP:4:ILE:HD12   | 2.14                     | 0.72              |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:HB3  | 1.70                     | 0.72              |
| 29:YF:32:LEU:HD12  | 29:YF:32:LEU:O     | 1.90                     | 0.72              |
| 29:YF:157:VAL:HB   | 29:YF:194:MET:HB3  | 1.70                     | 0.72              |
| 39:YT:117:ASP:O    | 39:YT:121:ILE:HG13 | 1.89                     | 0.72              |
| 47:Y1:3:LYS:HD3    | 47:Y1:43:TYR:HD2   | 1.52                     | 0.72              |
| 53:Y7:10:ARG:O     | 53:Y7:14:LYS:HB2   | 1.89                     | 0.72              |
| 1:QA:522:C:H41     | 12:QL:53:ARG:HH22  | 1.38                     | 0.72              |
| 2:QB:21:ARG:O      | 2:QB:23:ARG:HD3    | 1.90                     | 0.72              |
| 6:QF:77:ARG:HB2    | 6:QF:77:ARG:HH11   | 1.53                     | 0.72              |
| 8:QH:20:TYR:HD1    | 8:QH:65:TYR:CD2    | 2.07                     | 0.72              |
| 10:QJ:49:VAL:HG22  | 14:QN:41:ARG:HB3   | 1.59                     | 0.72              |
| 35:RP:29:LYS:HD2   | 35:RP:30:THR:HG22  | 1.72                     | 0.72              |
| 40:RU:69:CYS:HB3   | 40:RU:106:PHE:HZ   | 1.55                     | 0.72              |
| 40:RU:98:LEU:HD23  | 40:RU:99:ALA:N     | 2.04                     | 0.72              |
| 52:R6:13:CYS:HA    | 52:R6:50:ARG:O     | 1.89                     | 0.72              |
| 54:R8:61:LEU:O     | 54:R8:62:LEU:HB2   | 1.88                     | 0.72              |
| 5:XE:76:ILE:HB     | 5:XE:77:PRO:HD2    | 1.72                     | 0.72              |
| 25:YA:2298:A:H62   | 25:YA:2318:G:H8    | 1.38                     | 0.72              |
| 31:YH:128:PRO:HD2  | 31:YH:129:THR:H    | 1.55                     | 0.72              |
| 42:YW:70:TYR:H     | 42:YW:70:TYR:HD2   | 1.36                     | 0.72              |
| 8:QH:10:LEU:N      | 8:QH:10:LEU:HD23   | 2.04                     | 0.72              |
| 10:QJ:75:ILE:HG13  | 10:QJ:76:ASN:N     | 2.05                     | 0.72              |
| 16:QP:60:LEU:HA    | 16:QP:64:ALA:HB3   | 1.71                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:29:ASN:H     | 29:RF:112:MET:HE1  | 1.54                     | 0.72              |
| 29:RF:32:LEU:HD12  | 29:RF:32:LEU:O     | 1.90                     | 0.72              |
| 31:RH:89:ILE:CD1   | 31:RH:129:THR:HB   | 2.19                     | 0.72              |
| 39:RT:11:GLU:CD    | 39:RT:11:GLU:N     | 2.47                     | 0.72              |
| 53:R7:10:ARG:O     | 53:R7:14:LYS:HB2   | 1.90                     | 0.72              |
| 1:XA:1314:C:OP1    | 19:XS:6:LYS:HE3    | 1.90                     | 0.72              |
| 12:XL:126:LYS:HB2  | 12:XL:126:LYS:NZ   | 2.04                     | 0.72              |
| 20:XT:97:ALA:O     | 20:XT:99:LEU:HD13  | 1.89                     | 0.72              |
| 28:YE:56:PRO:O     | 28:YE:57:LYS:HB2   | 1.89                     | 0.72              |
| 28:YE:197:ILE:HD11 | 28:YE:199:ARG:HH12 | 1.55                     | 0.72              |
| 31:YH:26:VAL:CG1   | 31:YH:27:LYS:H     | 2.02                     | 0.72              |
| 44:YY:57:GLN:HE21  | 44:YY:58:GLY:H     | 1.37                     | 0.72              |
| 10:QJ:98:ILE:H     | 10:QJ:98:ILE:HD12  | 1.55                     | 0.72              |
| 13:QM:49:THR:HG22  | 13:QM:51:ALA:N     | 2.01                     | 0.72              |
| 25:RA:1080:C:N4    | 25:RA:1088:A:OP2   | 2.23                     | 0.72              |
| 31:RH:152:ARG:O    | 31:RH:153:LYS:HD2  | 1.90                     | 0.72              |
| 35:RP:114:ILE:HD13 | 35:RP:125:VAL:HG21 | 1.72                     | 0.72              |
| 36:RQ:79:LEU:O     | 36:RQ:79:LEU:CD2   | 2.36                     | 0.72              |
| 37:RR:117:VAL:HG22 | 37:RR:118:GLU:N    | 2.05                     | 0.72              |
| 40:RU:66:ASN:HB2   | 40:RU:76:TYR:HB2   | 1.72                     | 0.72              |
| 44:RY:51:VAL:HG13  | 44:RY:52:SER:N     | 2.03                     | 0.72              |
| 54:R8:60:LEU:O     | 54:R8:63:PRO:HD2   | 1.90                     | 0.72              |
| 8:XH:10:LEU:HD23   | 8:XH:10:LEU:N      | 2.04                     | 0.72              |
| 10:XJ:98:ILE:H     | 10:XJ:98:ILE:HD12  | 1.55                     | 0.72              |
| 15:XO:79:ARG:O     | 15:XO:82:ILE:HG22  | 1.89                     | 0.72              |
| 25:YA:2713:A:OP1   | 37:YR:14:SER:OG    | 2.08                     | 0.72              |
| 28:YE:13:ARG:HA    | 28:YE:22:PRO:HA    | 1.71                     | 0.72              |
| 29:YF:9:ILE:HD11   | 29:YF:125:LEU:HG   | 1.70                     | 0.72              |
| 31:YH:30:LYS:HD2   | 31:YH:81:GLU:H     | 1.54                     | 0.72              |
| 31:YH:84:SER:O     | 31:YH:85:LYS:HB2   | 1.89                     | 0.72              |
| 25:RA:2404:C:H1'   | 35:RP:67:MET:HE1   | 1.72                     | 0.71              |
| 37:RR:3:HIS:O      | 37:RR:5:LYS:N      | 2.22                     | 0.71              |
| 37:RR:85:PRO:O     | 37:RR:87:TYR:N     | 2.22                     | 0.71              |
| 38:RS:26:LEU:O     | 38:RS:26:LEU:HD23  | 1.90                     | 0.71              |
| 39:RT:102:ILE:HB   | 39:RT:110:ILE:CD1  | 2.19                     | 0.71              |
| 52:R6:7:ILE:C      | 52:R6:9:LEU:H      | 1.98                     | 0.71              |
| 53:R7:5:TRP:NE1    | 53:R7:7:PRO:HG3    | 2.04                     | 0.71              |
| 2:XB:168:THR:HB    | 2:XB:192:SER:HB2   | 1.70                     | 0.71              |
| 10:XJ:5:ARG:HG3    | 10:XJ:71:LEU:HD11  | 1.72                     | 0.71              |
| 25:YA:270(R):G:N3  | 47:Y1:78:LYS:NZ    | 2.37                     | 0.71              |
| 25:YA:1803:A:H4'   | 27:YD:259:THR:CG2  | 2.20                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Y1:76:ARG:HH11  | 47:Y1:76:ARG:HG2   | 1.54                     | 0.71              |
| 1:QA:953:G:H5'     | 1:QA:965:A:H61     | 1.55                     | 0.71              |
| 2:QB:187:LEU:HD11  | 2:QB:204:ASN:O     | 1.91                     | 0.71              |
| 20:QT:57:ARG:HD3   | 20:QT:102:GLY:O    | 1.90                     | 0.71              |
| 25:RA:1264:G:H5'   | 51:R5:11:THR:HG21  | 1.71                     | 0.71              |
| 25:RA:2014:A:O2'   | 51:R5:2:ALA:HB2    | 1.90                     | 0.71              |
| 28:RE:93:VAL:H     | 28:RE:95:ILE:HD12  | 1.54                     | 0.71              |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:HH12 | 1.55                     | 0.71              |
| 30:RG:7:LEU:HD21   | 30:RG:176:LEU:HD22 | 1.70                     | 0.71              |
| 40:RU:8:VAL:HG23   | 40:RU:11:ARG:NH2   | 1.99                     | 0.71              |
| 48:R2:29:LYS:HD3   | 48:R2:57:ILE:HD13  | 1.71                     | 0.71              |
| 19:XS:40:ILE:HG13  | 19:XS:44:MET:SD    | 2.31                     | 0.71              |
| 34:YO:3:GLN:HB2    | 34:YO:4:PRO:HD2    | 1.72                     | 0.71              |
| 35:YP:85:LEU:HA    | 35:YP:88:LEU:HD22  | 1.71                     | 0.71              |
| 38:YS:83:LYS:HG2   | 38:YS:109:GLY:N    | 2.04                     | 0.71              |
| 40:YU:69:CYS:HB3   | 40:YU:106:PHE:HZ   | 1.55                     | 0.71              |
| 51:Y5:2:ALA:O      | 51:Y5:3:LYS:HB2    | 1.88                     | 0.71              |
| 19:QS:40:ILE:HG13  | 19:QS:44:MET:SD    | 2.30                     | 0.71              |
| 20:QT:83:ARG:HA    | 20:QT:86:ARG:HB3   | 1.71                     | 0.71              |
| 25:RA:2114:A:N6    | 25:RA:2119:A:N7    | 2.39                     | 0.71              |
| 34:RO:3:GLN:HB2    | 34:RO:4:PRO:HD2    | 1.72                     | 0.71              |
| 35:RP:85:LEU:HA    | 35:RP:88:LEU:HD22  | 1.71                     | 0.71              |
| 36:RQ:81:VAL:C     | 36:RQ:82:ARG:HG2   | 2.14                     | 0.71              |
| 38:RS:83:LYS:HG2   | 38:RS:109:GLY:N    | 2.04                     | 0.71              |
| 6:XF:25:ILE:HD13   | 6:XF:28:ARG:NH1    | 2.05                     | 0.71              |
| 16:XP:45:THR:HG23  | 16:XP:46:PRO:HD2   | 1.70                     | 0.71              |
| 20:XT:83:ARG:HA    | 20:XT:86:ARG:HB3   | 1.71                     | 0.71              |
| 25:YA:503:A:H4'    | 25:YA:504:U:H5'    | 1.71                     | 0.71              |
| 29:YF:185:ASP:OD1  | 29:YF:188:ARG:NH1  | 2.23                     | 0.71              |
| 38:YS:67:ARG:O     | 38:YS:71:ARG:HG3   | 1.90                     | 0.71              |
| 38:YS:103:GLU:O    | 38:YS:106:ARG:HG3  | 1.90                     | 0.71              |
| 42:YW:1:MET:HA     | 42:YW:1:MET:HE3    | 1.71                     | 0.71              |
| 52:Y6:28:ARG:HB3   | 52:Y6:30:THR:H     | 1.55                     | 0.71              |
| 54:Y8:58:ILE:HD13  | 54:Y8:61:LEU:HD11  | 1.72                     | 0.71              |
| 54:Y8:60:LEU:O     | 54:Y8:63:PRO:HD2   | 1.90                     | 0.71              |
| 4:QD:25:ARG:HH12   | 4:QD:30:LYS:HE3    | 1.56                     | 0.71              |
| 10:QJ:49:VAL:O     | 10:QJ:60:ARG:HB3   | 1.90                     | 0.71              |
| 25:RA:1061:U:H5'   | 25:RA:1070:A:H1'   | 1.71                     | 0.71              |
| 27:RD:244:ARG:HB2  | 27:RD:245:PRO:HD2  | 1.71                     | 0.71              |
| 35:RP:49:ARG:HD2   | 54:R8:58:ILE:CG2   | 2.20                     | 0.71              |
| 38:RS:67:ARG:O     | 38:RS:71:ARG:HG3   | 1.89                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:963:G:N3     | 10:XJ:55:LYS:NZ    | 2.36                     | 0.71              |
| 2:XB:214:ILE:HA   | 2:XB:217:ARG:HH21  | 1.55                     | 0.71              |
| 3:XC:16:ARG:HD2   | 3:XC:54:ARG:NH2    | 2.03                     | 0.71              |
| 20:XT:63:ILE:HG22 | 20:XT:77:ALA:HB1   | 1.73                     | 0.71              |
| 25:YA:2023:G:H5'  | 25:YA:2617:C:H4'   | 1.72                     | 0.71              |
| 29:YF:185:ASP:HA  | 29:YF:188:ARG:CD   | 2.20                     | 0.71              |
| 35:YP:58:THR:O    | 35:YP:61:ARG:CZ    | 2.38                     | 0.71              |
| 53:Y7:5:TRP:NE1   | 53:Y7:7:PRO:HG3    | 2.04                     | 0.71              |
| 28:RE:21:VAL:HB   | 28:RE:22:PRO:CB    | 2.18                     | 0.71              |
| 41:RV:39:LEU:O    | 41:RV:40:LEU:HD23  | 1.90                     | 0.71              |
| 43:RX:12:VAL:HG12 | 43:RX:27:THR:O     | 1.91                     | 0.71              |
| 4:XD:20:TYR:CE2   | 4:XD:27:TYR:HE2    | 2.09                     | 0.71              |
| 25:YA:64:A:C4     | 43:YX:66:LEU:HD13  | 2.24                     | 0.71              |
| 27:YD:263:ARG:HB2 | 27:YD:263:ARG:NH1  | 2.06                     | 0.71              |
| 1:QA:1073:U:O2'   | 2:QB:104:ASN:OD1   | 2.09                     | 0.71              |
| 2:QB:59:GLU:O     | 2:QB:62:ALA:HB3    | 1.90                     | 0.71              |
| 7:QG:8:GLU:CD     | 7:QG:8:GLU:H       | 1.97                     | 0.71              |
| 25:RA:83:G:N2     | 25:RA:103:A:OP2    | 2.23                     | 0.71              |
| 25:RA:2667:C:H1'  | 31:RH:109:PHE:HD2  | 1.56                     | 0.71              |
| 26:RB:42:C:N4     | 30:RG:91:ARG:HH21  | 1.87                     | 0.71              |
| 7:XG:78:ARG:HH12  | 7:XG:80:VAL:CG2    | 2.04                     | 0.71              |
| 25:YA:666:G:H4'   | 35:YP:49:ARG:NH1   | 2.05                     | 0.71              |
| 25:YA:742:G:H2'   | 25:YA:743:G:H8     | 1.55                     | 0.71              |
| 25:YA:2562:U:O2'  | 34:YO:23:ARG:NH1   | 2.22                     | 0.71              |
| 32:YI:21:VAL:HG21 | 32:YI:25:TYR:HD1   | 1.56                     | 0.71              |
| 36:YQ:81:VAL:C    | 36:YQ:82:ARG:HG2   | 2.15                     | 0.71              |
| 44:YY:89:PHE:C    | 44:YY:90:LEU:HD13  | 2.15                     | 0.71              |
| 52:Y6:36:LEU:HD13 | 52:Y6:50:ARG:NH1   | 2.05                     | 0.71              |
| 8:QH:41:ARG:HH11  | 8:QH:41:ARG:CB     | 2.03                     | 0.71              |
| 19:QS:5:LEU:CD2   | 50:R4:67:TYR:CE2   | 2.73                     | 0.71              |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:OH    | 1.90                     | 0.71              |
| 38:RS:106:ARG:CA  | 38:RS:110:LEU:HD11 | 2.19                     | 0.71              |
| 50:R4:29:PRO:O    | 50:R4:30:GLU:HB2   | 1.89                     | 0.71              |
| 52:R6:25:LYS:HD2  | 54:R8:34:TRP:HZ2   | 1.56                     | 0.71              |
| 15:XO:71:GLN:HB2  | 15:XO:78:TYR:CD1   | 2.24                     | 0.71              |
| 15:XO:87:ILE:HG22 | 15:XO:88:ARG:N     | 2.00                     | 0.71              |
| 20:XT:27:LYS:O    | 20:XT:30:LYS:HB3   | 1.89                     | 0.71              |
| 20:XT:57:ARG:HD3  | 20:XT:102:GLY:O    | 1.90                     | 0.71              |
| 28:YE:93:VAL:H    | 28:YE:95:ILE:HD12  | 1.54                     | 0.71              |
| 10:QJ:5:ARG:HG3   | 10:QJ:71:LEU:HD11  | 1.72                     | 0.71              |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CG    | 2.25                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:265:A:N6     | 25:RA:427:U:O2'    | 2.23                     | 0.71              |
| 25:RA:2470:G:H5'   | 36:RQ:56:ARG:HH22  | 1.56                     | 0.71              |
| 29:RF:178:PRO:HB2  | 29:RF:201:VAL:HG11 | 1.73                     | 0.71              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:HG3  | 1.70                     | 0.71              |
| 52:R6:36:LEU:HD13  | 52:R6:50:ARG:NH1   | 2.05                     | 0.71              |
| 11:XK:124:LYS:HD2  | 11:XK:125:PHE:CE1  | 2.25                     | 0.71              |
| 28:YE:174:ASP:CG   | 28:YE:175:VAL:H    | 1.98                     | 0.71              |
| 39:YT:23:ARG:HB2   | 39:YT:24:PRO:HD2   | 1.70                     | 0.71              |
| 43:YX:12:VAL:HG12  | 43:YX:27:THR:O     | 1.91                     | 0.71              |
| 45:YZ:145:GLU:HG3  | 45:YZ:146:ILE:HG12 | 1.72                     | 0.71              |
| 1:QA:1288:A:N3     | 1:QA:1352:C:O2'    | 2.24                     | 0.71              |
| 2:QB:75:LYS:O      | 2:QB:75:LYS:HD3    | 1.89                     | 0.71              |
| 25:RA:2112:G:O6    | 25:RA:2169:A:N6    | 2.24                     | 0.71              |
| 27:RD:263:ARG:HB2  | 27:RD:263:ARG:NH1  | 2.05                     | 0.71              |
| 35:RP:83:VAL:CG1   | 35:RP:112:LEU:HD21 | 2.21                     | 0.71              |
| 44:RY:89:PHE:C     | 44:RY:90:LEU:HD13  | 2.15                     | 0.71              |
| 54:R8:58:ILE:HD13  | 54:R8:61:LEU:HD11  | 1.72                     | 0.71              |
| 1:XA:1199:U:H4'    | 10:XJ:54:PHE:CZ    | 2.26                     | 0.71              |
| 2:XB:59:GLU:O      | 2:XB:62:ALA:HB3    | 1.90                     | 0.71              |
| 2:XB:126:GLU:CG    | 2:XB:129:GLU:HG3   | 2.20                     | 0.71              |
| 11:XK:48:ILE:HD12  | 11:XK:63:LEU:HB3   | 1.71                     | 0.71              |
| 25:YA:443:A:C5     | 29:YF:45:ARG:HD2   | 2.26                     | 0.71              |
| 25:YA:1826:G:H4'   | 27:YD:242:ARG:HH21 | 1.54                     | 0.71              |
| 35:YP:49:ARG:HD2   | 54:Y8:58:ILE:CG2   | 2.20                     | 0.71              |
| 38:YS:83:LYS:HZ1   | 38:YS:109:GLY:HA2  | 1.52                     | 0.71              |
| 48:Y2:7:ARG:HG3    | 48:Y2:7:ARG:HH11   | 1.55                     | 0.71              |
| 51:Y5:40:LYS:HE2   | 51:Y5:47:PRO:HD2   | 1.73                     | 0.71              |
| 3:QC:16:ARG:HB2    | 3:QC:16:ARG:NH1    | 2.04                     | 0.71              |
| 8:QH:84:ARG:HH12   | 8:QH:86:ILE:CD1    | 2.02                     | 0.71              |
| 11:QK:124:LYS:HD2  | 11:QK:125:PHE:CE1  | 2.25                     | 0.71              |
| 13:QM:121:LYS:HE2  | 13:QM:121:LYS:CA   | 2.21                     | 0.71              |
| 18:QR:56:THR:HB    | 18:QR:58:LEU:HD12  | 1.71                     | 0.71              |
| 20:QT:23:ARG:CA    | 20:QT:26:ASN:HD21  | 2.04                     | 0.71              |
| 25:RA:1542:G:O6    | 25:RA:1543:A:C6    | 2.43                     | 0.71              |
| 25:RA:2693:A:H2'   | 25:RA:2694:G:H8    | 1.56                     | 0.71              |
| 29:RF:185:ASP:OD1  | 29:RF:188:ARG:NH1  | 2.24                     | 0.71              |
| 2:XB:172:ILE:H     | 2:XB:172:ILE:HD12  | 1.56                     | 0.71              |
| 3:XC:123:GLN:O     | 3:XC:128:PHE:HB2   | 1.91                     | 0.71              |
| 20:XT:23:ARG:CA    | 20:XT:26:ASN:HD21  | 2.03                     | 0.71              |
| 25:YA:443:A:N7     | 29:YF:45:ARG:HD2   | 2.05                     | 0.71              |
| 25:YA:518:G:H4'    | 42:YW:18:ARG:NH1   | 2.00                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1279:G:H4'   | 37:YR:31:HIS:HD2   | 1.56                     | 0.71              |
| 25:YA:2701:C:H3'   | 25:YA:2702:U:C5'   | 2.19                     | 0.71              |
| 25:YA:2810:A:O3'   | 28:YE:61:ARG:HG3   | 1.90                     | 0.71              |
| 42:YW:6:ILE:HG12   | 42:YW:104:THR:HG23 | 1.73                     | 0.71              |
| 2:QB:8:LYS:HD3     | 2:QB:8:LYS:N       | 2.02                     | 0.70              |
| 5:QE:78:HIS:HA     | 8:QH:105:ARG:HB2   | 1.72                     | 0.70              |
| 28:RE:174:ASP:CG   | 28:RE:175:VAL:H    | 1.98                     | 0.70              |
| 29:RF:66:PRO:O     | 29:RF:67:GLN:HB3   | 1.89                     | 0.70              |
| 29:RF:101:LEU:O    | 29:RF:106:ARG:NH1  | 2.23                     | 0.70              |
| 31:RH:132:ARG:HH11 | 31:RH:132:ARG:CB   | 1.97                     | 0.70              |
| 3:XC:152:ILE:HB    | 3:XC:199:LYS:HB2   | 1.73                     | 0.70              |
| 10:XJ:81:THR:C     | 10:XJ:83:GLU:H     | 1.99                     | 0.70              |
| 15:XO:65:ARG:HB2   | 15:XO:65:ARG:HH11  | 1.56                     | 0.70              |
| 34:YO:113:LYS:HG2  | 34:YO:117:LEU:HD11 | 1.71                     | 0.70              |
| 52:Y6:29:ASN:OD1   | 52:Y6:30:THR:HG22  | 1.91                     | 0.70              |
| 4:QD:190:ASP:HB3   | 4:QD:193:ASP:OD1   | 1.91                     | 0.70              |
| 27:RD:43:ARG:HB3   | 27:RD:54:ARG:HB2   | 1.73                     | 0.70              |
| 35:RP:58:THR:O     | 35:RP:61:ARG:CZ    | 2.38                     | 0.70              |
| 41:RV:51:VAL:HG12  | 41:RV:52:VAL:N     | 2.06                     | 0.70              |
| 54:R8:29:LYS:HD3   | 54:R8:44:LYS:HB2   | 1.71                     | 0.70              |
| 2:XB:132:LYS:HA    | 2:XB:135:GLN:HB2   | 1.71                     | 0.70              |
| 9:XI:15:ALA:HA     | 9:XI:64:THR:O      | 1.91                     | 0.70              |
| 12:XL:24:VAL:HG12  | 12:XL:24:VAL:O     | 1.91                     | 0.70              |
| 13:XM:4:ILE:N      | 13:XM:9:ILE:HG21   | 2.06                     | 0.70              |
| 13:XM:121:LYS:HE2  | 13:XM:121:LYS:HA   | 1.71                     | 0.70              |
| 29:YF:66:PRO:O     | 29:YF:67:GLN:HB3   | 1.89                     | 0.70              |
| 31:YH:80:SER:O     | 31:YH:81:GLU:HB2   | 1.89                     | 0.70              |
| 1:QA:1192:C:O2     | 5:QE:25:ARG:NH2    | 2.23                     | 0.70              |
| 2:QB:126:GLU:CG    | 2:QB:129:GLU:HG3   | 2.20                     | 0.70              |
| 4:QD:166:LYS:HD3   | 27:YD:134:ARG:HH11 | 1.55                     | 0.70              |
| 20:QT:63:ILE:HG22  | 20:QT:77:ALA:HB1   | 1.73                     | 0.70              |
| 29:RF:164:ARG:HG3  | 29:RF:175:THR:OG1  | 1.92                     | 0.70              |
| 2:XB:187:LEU:HD11  | 2:XB:204:ASN:O     | 1.90                     | 0.70              |
| 5:XE:11:ILE:HD11   | 5:XE:31:LEU:CD1    | 2.17                     | 0.70              |
| 10:XJ:6:ILE:HG13   | 10:XJ:72:VAL:O     | 1.91                     | 0.70              |
| 28:YE:14:ILE:HG12  | 28:YE:15:PHE:N     | 2.06                     | 0.70              |
| 29:YF:101:LEU:O    | 29:YF:106:ARG:NH1  | 2.23                     | 0.70              |
| 40:YU:66:ASN:HB2   | 40:YU:76:TYR:HB2   | 1.72                     | 0.70              |
| 5:QE:78:HIS:HE1    | 5:QE:143:ARG:H     | 1.38                     | 0.70              |
| 9:QI:15:ALA:HA     | 9:QI:64:THR:O      | 1.91                     | 0.70              |
| 10:QJ:6:ILE:HG13   | 10:QJ:72:VAL:O     | 1.91                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:244:ARG:HB2  | 27:YD:245:PRO:HD2  | 1.72                     | 0.70              |
| 29:YF:178:PRO:HG2  | 29:YF:179:GLU:OE2  | 1.90                     | 0.70              |
| 31:YH:59:ARG:HH11  | 31:YH:59:ARG:HG3   | 1.56                     | 0.70              |
| 31:YH:89:ILE:CD1   | 31:YH:129:THR:HB   | 2.20                     | 0.70              |
| 31:YH:152:ARG:O    | 31:YH:153:LYS:CB   | 2.39                     | 0.70              |
| 35:YP:20:GLY:HA2   | 35:YP:27:HIS:O     | 1.92                     | 0.70              |
| 2:QB:214:ILE:HA    | 2:QB:217:ARG:HH21  | 1.55                     | 0.70              |
| 25:RA:1483:G:O6    | 25:RA:1506:C:N4    | 2.22                     | 0.70              |
| 25:RA:2286:A:OP1   | 52:R6:28:ARG:NE    | 2.24                     | 0.70              |
| 31:RH:128:PRO:HD2  | 31:RH:129:THR:H    | 1.55                     | 0.70              |
| 31:RH:154:PRO:O    | 31:RH:155:SER:HB2  | 1.91                     | 0.70              |
| 36:RQ:32:TYR:CD1   | 36:RQ:133:ARG:HA   | 2.27                     | 0.70              |
| 44:RY:45:VAL:HG12  | 44:RY:60:PHE:CD1   | 2.27                     | 0.70              |
| 48:R2:7:ARG:HH11   | 48:R2:7:ARG:HG3    | 1.55                     | 0.70              |
| 51:R5:40:LYS:HE2   | 51:R5:47:PRO:HD2   | 1.73                     | 0.70              |
| 52:R6:29:ASN:OD1   | 52:R6:30:THR:HG22  | 1.91                     | 0.70              |
| 1:XA:1305:G:N2     | 1:XA:1331:G:H2'    | 2.06                     | 0.70              |
| 6:XF:72:VAL:CG2    | 6:XF:90:VAL:HG11   | 2.20                     | 0.70              |
| 31:YH:86:GLU:CG    | 31:YH:165:ALA:H    | 1.94                     | 0.70              |
| 31:YH:103:LEU:HD12 | 31:YH:131:VAL:HG21 | 1.73                     | 0.70              |
| 40:YU:65:ILE:HG12  | 40:YU:96:ALA:HB1   | 1.73                     | 0.70              |
| 41:YV:22:VAL:HG12  | 41:YV:23:GLU:N     | 2.06                     | 0.70              |
| 47:Y1:7:ILE:CD1    | 47:Y1:70:VAL:HG22  | 2.21                     | 0.70              |
| 52:Y6:25:LYS:HD2   | 54:Y8:34:TRP:HZ2   | 1.56                     | 0.70              |
| 25:RA:1012:U:H3    | 33:RN:25:ARG:HH11  | 1.40                     | 0.70              |
| 25:RA:1543:A:O2'   | 25:RA:1544:C:H3'   | 1.91                     | 0.70              |
| 25:RA:1754:C:OP1   | 39:RT:96:ARG:NH1   | 2.21                     | 0.70              |
| 33:RN:89:LYS:O     | 33:RN:93:THR:HG22  | 1.90                     | 0.70              |
| 38:RS:54:LEU:HD13  | 38:RS:54:LEU:O     | 1.91                     | 0.70              |
| 38:RS:83:LYS:HZ1   | 38:RS:109:GLY:HA2  | 1.56                     | 0.70              |
| 5:XE:82:VAL:HG12   | 5:XE:83:GLU:N      | 2.06                     | 0.70              |
| 13:XM:121:LYS:HE2  | 13:XM:121:LYS:CA   | 2.21                     | 0.70              |
| 28:YE:28:ALA:HB3   | 28:YE:93:VAL:HG22  | 1.72                     | 0.70              |
| 29:YF:164:ARG:HG3  | 29:YF:175:THR:OG1  | 1.91                     | 0.70              |
| 36:YQ:32:TYR:CD1   | 36:YQ:133:ARG:HA   | 2.27                     | 0.70              |
| 39:YT:41:ARG:NH2   | 39:YT:43:GLN:HB2   | 2.06                     | 0.70              |
| 47:Y1:81:LYS:HE2   | 47:Y1:81:LYS:CA    | 2.13                     | 0.70              |
| 1:QA:192:U:H4'     | 20:QT:102:GLY:O    | 1.92                     | 0.70              |
| 5:QE:76:ILE:HB     | 5:QE:77:PRO:HD2    | 1.72                     | 0.70              |
| 25:RA:583:G:H5''   | 40:RU:10:ARG:HH12  | 1.55                     | 0.70              |
| 29:RF:65:TRP:HZ3   | 29:RF:73:ALA:O     | 1.74                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:152:ARG:O   | 31:RH:153:LYS:CB   | 2.39                     | 0.70              |
| 31:RH:154:PRO:HG2 | 31:RH:162:ILE:O    | 1.92                     | 0.70              |
| 44:RY:57:GLN:HE21 | 44:RY:58:GLY:H     | 1.37                     | 0.70              |
| 1:XA:1151:A:H1'   | 10:XJ:39:PRO:HB2   | 1.72                     | 0.70              |
| 2:XB:101:MET:HA   | 2:XB:108:ILE:CG1   | 2.14                     | 0.70              |
| 2:XB:162:ILE:HD11 | 2:XB:184:VAL:HG13  | 1.74                     | 0.70              |
| 8:XH:49:GLU:HG3   | 8:XH:51:VAL:HG13   | 1.74                     | 0.70              |
| 17:XQ:4:LYS:CE    | 17:XQ:6:LEU:HD21   | 2.20                     | 0.70              |
| 25:YA:1980:G:O2'  | 25:YA:1982:C:OP2   | 2.08                     | 0.70              |
| 27:YD:43:ARG:HB3  | 27:YD:54:ARG:HB2   | 1.73                     | 0.70              |
| 31:YH:154:PRO:HG2 | 31:YH:162:ILE:O    | 1.91                     | 0.70              |
| 42:YW:29:LEU:HD21 | 42:YW:33:ARG:CZ    | 2.22                     | 0.70              |
| 51:Y5:40:LYS:HE2  | 51:Y5:47:PRO:CD    | 2.21                     | 0.70              |
| 5:QE:82:VAL:HG12  | 5:QE:83:GLU:N      | 2.06                     | 0.70              |
| 25:RA:2208:U:H1'  | 27:RD:151:LYS:HE2  | 1.74                     | 0.70              |
| 29:RF:178:PRO:HG2 | 29:RF:179:GLU:OE2  | 1.90                     | 0.70              |
| 47:R1:7:ILE:CD1   | 47:R1:70:VAL:HG22  | 2.21                     | 0.70              |
| 4:XD:190:ASP:HB3  | 4:XD:193:ASP:OD1   | 1.91                     | 0.70              |
| 25:YA:573:G:N1    | 25:YA:2031:A:OP2   | 2.23                     | 0.70              |
| 25:YA:1509:C:H3'  | 25:YA:1510:A:H5''  | 1.74                     | 0.70              |
| 26:YB:15:A:H5'    | 26:YB:16:G:C8      | 2.27                     | 0.70              |
| 26:YB:42:C:N4     | 30:YG:91:ARG:HH21  | 1.89                     | 0.70              |
| 29:YF:178:PRO:HB2 | 29:YF:201:VAL:HG11 | 1.73                     | 0.70              |
| 34:YO:63:VAL:HG13 | 34:YO:84:ALA:HA    | 1.73                     | 0.70              |
| 38:YS:42:ASP:O    | 38:YS:43:GLU:HB2   | 1.90                     | 0.70              |
| 1:QA:1071:C:H5''  | 5:QE:49:PRO:HG2    | 1.74                     | 0.70              |
| 3:QC:152:ILE:HB   | 3:QC:199:LYS:HB2   | 1.72                     | 0.70              |
| 16:QP:14:ASN:N    | 16:QP:15:PRO:HD3   | 2.07                     | 0.70              |
| 17:QQ:52:LYS:HD2  | 17:QQ:55:ASP:OD1   | 1.91                     | 0.70              |
| 27:RD:65:ILE:HD13 | 27:RD:65:ILE:O     | 1.92                     | 0.70              |
| 36:RQ:59:ARG:C    | 36:RQ:60:ARG:HG3   | 2.17                     | 0.70              |
| 42:RW:29:LEU:HD21 | 42:RW:33:ARG:CZ    | 2.22                     | 0.70              |
| 47:R1:82:LEU:HD13 | 47:R1:83:GLU:N     | 2.05                     | 0.70              |
| 1:XA:1152:A:H5''  | 10:XJ:13:HIS:HD2   | 1.57                     | 0.70              |
| 20:XT:50:GLU:HG3  | 20:XT:51:GLU:H     | 1.54                     | 0.70              |
| 25:YA:583:G:H5''  | 40:YU:10:ARG:HH12  | 1.57                     | 0.70              |
| 30:YG:131:TYR:O   | 30:YG:159:VAL:HG13 | 1.92                     | 0.70              |
| 41:YV:41:GLY:HA3  | 41:YV:46:VAL:HG11  | 1.74                     | 0.70              |
| 41:YV:51:VAL:HG12 | 41:YV:52:VAL:N     | 2.06                     | 0.70              |
| 13:QM:4:ILE:N     | 13:QM:9:ILE:HG21   | 2.06                     | 0.70              |
| 19:QS:5:LEU:HD22  | 50:R4:67:TYR:CE2   | 2.26                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:QS:51:VAL:O     | 19:QS:57:HIS:HA    | 1.92                     | 0.70              |
| 27:RD:65:ILE:HD11  | 27:RD:67:PHE:CD1   | 2.27                     | 0.70              |
| 31:RH:150:ALA:C    | 31:RH:152:ARG:N    | 2.44                     | 0.70              |
| 38:RS:106:ARG:N    | 38:RS:110:LEU:HD21 | 2.07                     | 0.70              |
| 40:RU:65:ILE:HG12  | 40:RU:96:ALA:HB1   | 1.73                     | 0.70              |
| 43:RX:57:LEU:HD11  | 43:RX:78:LYS:HD2   | 1.73                     | 0.70              |
| 2:XB:95:GLN:HE21   | 2:XB:147:LYS:HE2   | 1.56                     | 0.70              |
| 3:XC:105:GLU:HG2   | 3:XC:106:VAL:H     | 1.57                     | 0.70              |
| 10:XJ:49:VAL:O     | 10:XJ:60:ARG:HB3   | 1.90                     | 0.70              |
| 27:YD:65:ILE:HD13  | 27:YD:65:ILE:O     | 1.91                     | 0.70              |
| 28:YE:103:ASP:OD1  | 28:YE:201:THR:HA   | 1.92                     | 0.70              |
| 35:YP:83:VAL:CG1   | 35:YP:112:LEU:HD21 | 2.21                     | 0.70              |
| 36:YQ:43:THR:OG1   | 36:YQ:46:GLN:HB2   | 1.91                     | 0.70              |
| 38:YS:54:LEU:HD13  | 38:YS:54:LEU:O     | 1.91                     | 0.70              |
| 43:YX:57:LEU:HD11  | 43:YX:78:LYS:HD2   | 1.73                     | 0.70              |
| 52:Y6:7:ILE:C      | 52:Y6:9:LEU:H      | 1.98                     | 0.70              |
| 3:QC:16:ARG:HD2    | 3:QC:54:ARG:NH2    | 2.03                     | 0.69              |
| 8:QH:87:SER:HB2    | 8:QH:93:VAL:HB     | 1.74                     | 0.69              |
| 30:RG:131:TYR:O    | 30:RG:159:VAL:HG13 | 1.92                     | 0.69              |
| 47:R1:7:ILE:HD12   | 47:R1:70:VAL:HG22  | 1.73                     | 0.69              |
| 8:XH:87:SER:HB2    | 8:XH:93:VAL:HB     | 1.74                     | 0.69              |
| 47:Y1:7:ILE:HD12   | 47:Y1:70:VAL:HG22  | 1.73                     | 0.69              |
| 47:Y1:82:LEU:HD12  | 47:Y1:83:GLU:CA    | 2.22                     | 0.69              |
| 2:QB:162:ILE:O     | 2:QB:162:ILE:HG13  | 1.92                     | 0.69              |
| 9:QI:113:LYS:HD2   | 9:QI:113:LYS:N     | 2.07                     | 0.69              |
| 10:QJ:38:ILE:O     | 10:QJ:38:ILE:HG13  | 1.91                     | 0.69              |
| 12:QL:24:VAL:HG12  | 12:QL:24:VAL:O     | 1.90                     | 0.69              |
| 27:RD:76:PRO:O     | 27:RD:98:VAL:HG23  | 1.91                     | 0.69              |
| 29:RF:108:LYS:HZ3  | 29:RF:108:LYS:HA   | 1.57                     | 0.69              |
| 47:R1:82:LEU:CD1   | 47:R1:83:GLU:C     | 2.64                     | 0.69              |
| 48:R2:47:ASN:O     | 48:R2:49:LYS:N     | 2.25                     | 0.69              |
| 14:XN:6:LEU:O      | 14:XN:6:LEU:HD23   | 1.92                     | 0.69              |
| 16:XP:14:ASN:N     | 16:XP:15:PRO:HD3   | 2.07                     | 0.69              |
| 35:YP:114:ILE:HD13 | 35:YP:125:VAL:HG21 | 1.72                     | 0.69              |
| 47:Y1:82:LEU:CD1   | 47:Y1:83:GLU:C     | 2.64                     | 0.69              |
| 4:QD:30:LYS:HD3    | 4:QD:30:LYS:H      | 1.57                     | 0.69              |
| 7:QG:78:ARG:HH12   | 7:QG:80:VAL:CG2    | 2.04                     | 0.69              |
| 21:QU:6:ARG:HE     | 21:QU:15:ARG:NE    | 1.90                     | 0.69              |
| 31:RH:59:ARG:HH11  | 31:RH:59:ARG:HG3   | 1.56                     | 0.69              |
| 31:RH:103:LEU:HD12 | 31:RH:131:VAL:HG21 | 1.73                     | 0.69              |
| 33:RN:46:VAL:O     | 33:RN:47:ALA:HB3   | 1.92                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:R1:82:LEU:HD12  | 47:R1:83:GLU:CA    | 2.21                     | 0.69              |
| 1:XA:797:C:OP1     | 11:XK:124:LYS:HE2  | 1.92                     | 0.69              |
| 1:XA:1443:G:N2     | 25:YA:2864:G:OP1   | 2.23                     | 0.69              |
| 12:XL:25:PRO:C     | 12:XL:27:LEU:H     | 1.98                     | 0.69              |
| 19:XS:51:VAL:O     | 19:XS:57:HIS:HA    | 1.92                     | 0.69              |
| 32:YI:144:VAL:HG13 | 32:YI:145:VAL:HG13 | 1.73                     | 0.69              |
| 48:Y2:47:ASN:O     | 48:Y2:49:LYS:N     | 2.25                     | 0.69              |
| 1:QA:377:G:OP1     | 16:QP:5:ARG:NH1    | 2.25                     | 0.69              |
| 2:QB:95:GLN:HE21   | 2:QB:147:LYS:HE2   | 1.56                     | 0.69              |
| 4:QD:120:LEU:HD22  | 4:QD:125:HIS:HB2   | 1.74                     | 0.69              |
| 15:QO:65:ARG:HB2   | 15:QO:65:ARG:HH11  | 1.57                     | 0.69              |
| 25:RA:2821:A:OP2   | 25:RA:2822:G:OP2   | 2.11                     | 0.69              |
| 28:RE:103:ASP:OD1  | 28:RE:201:THR:HA   | 1.92                     | 0.69              |
| 29:RF:103:LYS:HA   | 29:RF:106:ARG:CG   | 2.21                     | 0.69              |
| 35:RP:20:GLY:HA2   | 35:RP:27:HIS:O     | 1.92                     | 0.69              |
| 35:RP:126:VAL:CG1  | 35:RP:147:LEU:HD21 | 2.16                     | 0.69              |
| 36:RQ:43:THR:OG1   | 36:RQ:46:GLN:HB2   | 1.91                     | 0.69              |
| 44:RY:2:ARG:HH11   | 44:RY:2:ARG:HG2    | 1.57                     | 0.69              |
| 47:R1:74:VAL:HG12  | 47:R1:74:VAL:O     | 1.93                     | 0.69              |
| 10:XJ:38:ILE:O     | 10:XJ:38:ILE:HG13  | 1.92                     | 0.69              |
| 10:XJ:54:PHE:C     | 10:XJ:55:LYS:HG3   | 2.17                     | 0.69              |
| 25:YA:2306:C:H2'   | 25:YA:2307:G:H21   | 1.57                     | 0.69              |
| 27:YD:65:ILE:HD11  | 27:YD:67:PHE:CD1   | 2.27                     | 0.69              |
| 35:YP:64:LYS:HB2   | 54:Y8:25:MET:CG    | 2.22                     | 0.69              |
| 41:YV:66:ARG:HH12  | 41:YV:88:ARG:NH1   | 1.90                     | 0.69              |
| 47:Y1:53:VAL:HG22  | 47:Y1:74:VAL:HG13  | 1.74                     | 0.69              |
| 3:QC:147:LYS:O     | 3:QC:203:PHE:HB3   | 1.92                     | 0.69              |
| 4:QD:188:LEU:HD23  | 4:QD:189:PRO:HD2   | 1.75                     | 0.69              |
| 25:RA:676:A:H8     | 25:RA:2069:G:H21   | 1.41                     | 0.69              |
| 31:RH:4:ILE:HG13   | 31:RH:6:ARG:NE     | 2.08                     | 0.69              |
| 47:R1:4:VAL:HG23   | 47:R1:10:LYS:O     | 1.92                     | 0.69              |
| 2:XB:162:ILE:O     | 2:XB:162:ILE:HG13  | 1.92                     | 0.69              |
| 6:XF:67:MET:HB2    | 6:XF:68:PRO:HD2    | 1.75                     | 0.69              |
| 29:YF:65:TRP:HZ3   | 29:YF:73:ALA:O     | 1.74                     | 0.69              |
| 32:YI:1:MET:HG3    | 32:YI:23:PRO:HB3   | 1.75                     | 0.69              |
| 34:YO:8:LEU:HD22   | 34:YO:8:LEU:N      | 2.08                     | 0.69              |
| 47:Y1:82:LEU:HD13  | 47:Y1:83:GLU:N     | 2.05                     | 0.69              |
| 48:Y2:40:SER:C     | 48:Y2:42:GLY:H     | 2.00                     | 0.69              |
| 2:QB:172:ILE:H     | 2:QB:172:ILE:HD12  | 1.56                     | 0.69              |
| 2:QB:212:GLN:NE2   | 2:QB:216:SER:HB2   | 2.08                     | 0.69              |
| 3:QC:123:GLN:O     | 3:QC:128:PHE:HB2   | 1.91                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:QF:3:ARG:HB3     | 6:QF:93:SER:HB2    | 1.74                     | 0.69              |
| 8:QH:31:PHE:CE2    | 8:QH:35:ILE:HD11   | 2.27                     | 0.69              |
| 28:RE:7:VAL:HG23   | 28:RE:8:LYS:N      | 2.07                     | 0.69              |
| 30:RG:56:ALA:HB2   | 30:RG:153:ARG:HE   | 1.57                     | 0.69              |
| 33:RN:120:LEU:HD11 | 33:RN:122:VAL:HG23 | 1.74                     | 0.69              |
| 34:RO:63:VAL:HG13  | 34:RO:84:ALA:HA    | 1.72                     | 0.69              |
| 41:RV:41:GLY:HA3   | 41:RV:46:VAL:HG11  | 1.74                     | 0.69              |
| 1:XA:1392:G:H21    | 1:XA:1502:A:H8     | 1.38                     | 0.69              |
| 4:XD:20:TYR:CE2    | 4:XD:27:TYR:CE2    | 2.80                     | 0.69              |
| 10:XJ:48:THR:HA    | 10:XJ:62:HIS:HB3   | 1.75                     | 0.69              |
| 17:XQ:52:LYS:HD2   | 17:XQ:55:ASP:OD1   | 1.91                     | 0.69              |
| 35:YP:50:ARG:HB3   | 35:YP:50:ARG:NH2   | 1.98                     | 0.69              |
| 35:YP:61:ARG:H     | 35:YP:61:ARG:HD2   | 1.58                     | 0.69              |
| 47:Y1:64:ALA:HA    | 47:Y1:67:ILE:HG13  | 1.75                     | 0.69              |
| 51:Y5:40:LYS:HG2   | 51:Y5:47:PRO:HD2   | 1.75                     | 0.69              |
| 52:Y6:14:THR:HG21  | 52:Y6:19:ARG:HH21  | 1.58                     | 0.69              |
| 3:QC:105:GLU:HG2   | 3:QC:106:VAL:H     | 1.58                     | 0.69              |
| 4:QD:79:PHE:C      | 4:QD:79:PHE:HD2    | 2.00                     | 0.69              |
| 8:QH:6:ILE:HD12    | 8:QH:6:ILE:N       | 2.08                     | 0.69              |
| 17:QQ:4:LYS:CE     | 17:QQ:6:LEU:HD21   | 2.21                     | 0.69              |
| 19:QS:68:GLY:HA3   | 50:R4:68:ARG:CG    | 2.23                     | 0.69              |
| 27:RD:89:SER:HB2   | 27:RD:159:ALA:HB2  | 1.75                     | 0.69              |
| 28:RE:65:GLY:HA2   | 28:RE:70:ALA:CB    | 2.23                     | 0.69              |
| 35:RP:39:LYS:CA    | 35:RP:45:LEU:HD11  | 2.23                     | 0.69              |
| 16:XP:1:MET:O      | 16:XP:24:ALA:HB2   | 1.92                     | 0.69              |
| 25:YA:1918:A:O2'   | 25:YA:1920:C:N4    | 2.26                     | 0.69              |
| 27:YD:89:SER:HB2   | 27:YD:159:ALA:HB2  | 1.75                     | 0.69              |
| 30:YG:28:VAL:HG23  | 30:YG:29:TRP:CD1   | 2.28                     | 0.69              |
| 31:YH:154:PRO:O    | 31:YH:155:SER:HB2  | 1.91                     | 0.69              |
| 2:QB:101:MET:HA    | 2:QB:108:ILE:CG1   | 2.14                     | 0.69              |
| 8:QH:49:GLU:HG3    | 8:QH:51:VAL:HG13   | 1.74                     | 0.69              |
| 10:QJ:54:PHE:C     | 10:QJ:55:LYS:HG3   | 2.18                     | 0.69              |
| 10:QJ:54:PHE:CZ    | 10:QJ:55:LYS:NZ    | 2.61                     | 0.69              |
| 25:RA:2023:G:H5'   | 25:RA:2617:C:H4'   | 1.75                     | 0.69              |
| 25:RA:2219:G:OP1   | 27:RD:172:TYR:OH   | 2.06                     | 0.69              |
| 25:RA:2344:U:C2    | 52:R6:37:ARG:HD3   | 2.27                     | 0.69              |
| 30:RG:171:ALA:O    | 30:RG:175:LEU:HG   | 1.93                     | 0.69              |
| 33:RN:7:LYS:HD3    | 33:RN:9:VAL:HA     | 1.75                     | 0.69              |
| 35:RP:64:LYS:HB2   | 54:R8:25:MET:CG    | 2.22                     | 0.69              |
| 38:RS:52:SER:O     | 38:RS:56:LEU:HD22  | 1.93                     | 0.69              |
| 40:RU:90:VAL:O     | 40:RU:92:ARG:N     | 2.26                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:RV:66:ARG:HH12  | 41:RV:88:ARG:NH1   | 1.90                     | 0.69              |
| 44:RY:29:GLU:HB3   | 44:RY:38:ILE:HG12  | 1.74                     | 0.69              |
| 47:R1:53:VAL:HG22  | 47:R1:74:VAL:HG13  | 1.74                     | 0.69              |
| 47:R1:81:LYS:HE2   | 47:R1:81:LYS:CA    | 2.13                     | 0.69              |
| 51:R5:4:HIS:HB3    | 51:R5:5:PRO:HD3    | 1.75                     | 0.69              |
| 51:R5:40:LYS:HE2   | 51:R5:47:PRO:CD    | 2.21                     | 0.69              |
| 4:XD:13:ARG:HA     | 4:XD:33:MET:HE3    | 1.74                     | 0.69              |
| 6:XF:100:ASN:ND2   | 18:XR:23:LYS:HE3   | 2.08                     | 0.69              |
| 8:XH:31:PHE:CE2    | 8:XH:35:ILE:HD11   | 2.27                     | 0.69              |
| 8:XH:84:ARG:HH12   | 8:XH:86:ILE:CD1    | 2.02                     | 0.69              |
| 14:XN:44:LEU:CD1   | 14:XN:53:LEU:HD13  | 2.23                     | 0.69              |
| 25:YA:1022:G:H22   | 25:YA:1142(A):A:H2 | 1.40                     | 0.69              |
| 25:YA:1103:A:H5'   | 25:YA:1104:C:H5    | 1.57                     | 0.69              |
| 25:YA:2867:G:HO2'  | 25:YA:2868:A:H8    | 1.37                     | 0.69              |
| 27:YD:76:PRO:O     | 27:YD:98:VAL:HG23  | 1.92                     | 0.69              |
| 28:YE:7:VAL:HG23   | 28:YE:8:LYS:N      | 2.07                     | 0.69              |
| 29:YF:67:GLN:O     | 29:YF:68:LYS:CB    | 2.39                     | 0.69              |
| 30:YG:16:ARG:HH21  | 30:YG:31:VAL:CG1   | 2.05                     | 0.69              |
| 31:YH:89:ILE:HG12  | 31:YH:89:ILE:O     | 1.92                     | 0.69              |
| 33:YN:7:LYS:HD3    | 33:YN:9:VAL:HA     | 1.75                     | 0.69              |
| 33:YN:68:GLU:HG2   | 33:YN:88:GLU:OE1   | 1.92                     | 0.69              |
| 33:YN:120:LEU:HD11 | 33:YN:122:VAL:HG23 | 1.74                     | 0.69              |
| 35:YP:29:LYS:HD2   | 35:YP:30:THR:HG22  | 1.72                     | 0.69              |
| 35:YP:62:LEU:HD22  | 35:YP:62:LEU:H     | 1.53                     | 0.69              |
| 35:YP:62:LEU:HD23  | 54:Y8:25:MET:HB2   | 1.74                     | 0.69              |
| 38:YS:106:ARG:CA   | 38:YS:110:LEU:HD11 | 2.19                     | 0.69              |
| 38:YS:106:ARG:N    | 38:YS:110:LEU:HD21 | 2.07                     | 0.69              |
| 44:YY:45:VAL:HG12  | 44:YY:60:PHE:CD1   | 2.27                     | 0.69              |
| 1:QA:339:C:OP2     | 34:RO:97:ARG:NH1   | 2.26                     | 0.69              |
| 12:QL:25:PRO:C     | 12:QL:27:LEU:H     | 1.98                     | 0.69              |
| 16:QP:1:MET:O      | 16:QP:24:ALA:HB2   | 1.93                     | 0.69              |
| 27:RD:35:LYS:HB3   | 27:RD:63:ARG:HA    | 1.75                     | 0.69              |
| 30:RG:28:VAL:HG23  | 30:RG:29:TRP:CD1   | 2.28                     | 0.69              |
| 33:RN:68:GLU:HG2   | 33:RN:88:GLU:OE1   | 1.92                     | 0.69              |
| 36:RQ:80:GLU:HG3   | 36:RQ:81:VAL:H     | 1.58                     | 0.69              |
| 39:RT:41:ARG:NH2   | 39:RT:43:GLN:HB2   | 2.06                     | 0.69              |
| 48:R2:23:LYS:O     | 48:R2:27:GLU:OE1   | 2.11                     | 0.69              |
| 51:R5:40:LYS:HG2   | 51:R5:47:PRO:HD2   | 1.75                     | 0.69              |
| 52:R6:28:ARG:HB3   | 52:R6:30:THR:H     | 1.56                     | 0.69              |
| 1:XA:1318:A:H4'    | 19:XS:11:VAL:HG11  | 1.73                     | 0.69              |
| 4:XD:79:PHE:C      | 4:XD:79:PHE:HD2    | 1.99                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:XI:113:LYS:HD2  | 9:XI:113:LYS:N     | 2.07                     | 0.69              |
| 20:XT:64:ASP:HA   | 20:XT:67:ALA:HB3   | 1.74                     | 0.69              |
| 27:YD:17:THR:HG22 | 27:YD:205:VAL:N    | 2.08                     | 0.69              |
| 40:YU:65:ILE:HD11 | 40:YU:93:LYS:HA    | 1.74                     | 0.69              |
| 43:YX:12:VAL:HG11 | 43:YX:27:THR:OG1   | 1.93                     | 0.69              |
| 50:Y4:37:SER:C    | 50:Y4:39:CYS:H     | 1.99                     | 0.69              |
| 3:QC:195:VAL:HG12 | 3:QC:196:LEU:N     | 2.07                     | 0.69              |
| 6:QF:100:ASN:ND2  | 18:QR:23:LYS:HE3   | 2.08                     | 0.69              |
| 8:QH:112:LEU:HA   | 8:QH:134:ILE:HG12  | 1.75                     | 0.69              |
| 9:QI:46:ALA:HA    | 9:QI:78:LYS:HB2    | 1.75                     | 0.69              |
| 20:QT:47:GLY:O    | 20:QT:49:ALA:N     | 2.20                     | 0.69              |
| 35:RP:61:ARG:HD2  | 35:RP:61:ARG:H     | 1.58                     | 0.69              |
| 41:RV:22:VAL:HG12 | 41:RV:23:GLU:N     | 2.06                     | 0.69              |
| 52:R6:14:THR:HG21 | 52:R6:19:ARG:HH21  | 1.58                     | 0.69              |
| 1:XA:538:G:H5''   | 12:XL:114:LYS:HB2  | 1.74                     | 0.69              |
| 14:YN:23:ARG:CZ   | 14:YN:30:ALA:HB2   | 2.22                     | 0.69              |
| 19:XS:31:ILE:HG23 | 19:XS:49:ILE:HA    | 1.75                     | 0.69              |
| 27:YD:17:THR:CG2  | 27:YD:204:ILE:HA   | 2.23                     | 0.69              |
| 37:YR:29:LEU:HD23 | 37:YR:79:LEU:HD12  | 1.75                     | 0.69              |
| 40:YU:8:VAL:HG23  | 40:YU:11:ARG:NH2   | 1.99                     | 0.69              |
| 7:QG:155:ARG:N    | 7:QG:155:ARG:HD3   | 2.07                     | 0.68              |
| 20:QT:64:ASP:HA   | 20:QT:67:ALA:HB3   | 1.74                     | 0.68              |
| 25:RA:2306:C:H3'  | 25:RA:2307:G:H5''  | 1.75                     | 0.68              |
| 25:RA:2867:G:O2'  | 25:RA:2868:A:H8    | 1.75                     | 0.68              |
| 40:RU:65:ILE:HD11 | 40:RU:93:LYS:HA    | 1.74                     | 0.68              |
| 42:RW:6:ILE:HG12  | 42:RW:104:THR:HG23 | 1.73                     | 0.68              |
| 1:XA:939:G:H5''   | 7:YG:102:ARG:HH22  | 1.57                     | 0.68              |
| 1:XA:1192:C:O2    | 5:XE:25:ARG:NH2    | 2.25                     | 0.68              |
| 2:XB:212:GLN:NE2  | 2:XB:216:SER:HB2   | 2.08                     | 0.68              |
| 25:YA:278:A:O2'   | 25:YA:279:C:O4'    | 2.11                     | 0.68              |
| 27:YD:35:LYS:HB3  | 27:YD:63:ARG:HA    | 1.75                     | 0.68              |
| 27:YD:122:ASP:CG  | 27:YD:123:ALA:H    | 2.00                     | 0.68              |
| 28:YE:65:GLY:HA2  | 28:YE:70:ALA:CB    | 2.23                     | 0.68              |
| 30:YG:56:ALA:HB2  | 30:YG:153:ARG:HE   | 1.57                     | 0.68              |
| 2:QB:162:ILE:HD11 | 2:QB:184:VAL:HG13  | 1.74                     | 0.68              |
| 30:RG:16:ARG:HH21 | 30:RG:31:VAL:CG1   | 2.06                     | 0.68              |
| 33:RN:131:GLN:CD  | 33:RN:132:ALA:H    | 2.01                     | 0.68              |
| 4:XD:96:LEU:HD22  | 4:XD:96:LEU:N      | 2.08                     | 0.68              |
| 5:XE:78:HIS:HE1   | 5:XE:143:ARG:H     | 1.37                     | 0.68              |
| 7:YG:155:ARG:HD3  | 7:YG:155:ARG:N     | 2.07                     | 0.68              |
| 8:XH:6:ILE:H      | 8:XH:6:ILE:CD1     | 2.06                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1952:A:OP1   | 34:YO:44:LYS:NZ    | 2.24                     | 0.68              |
| 36:YQ:88:GLY:C     | 36:YQ:90:VAL:N     | 2.47                     | 0.68              |
| 38:YS:57:LYS:HD3   | 38:YS:57:LYS:H     | 1.58                     | 0.68              |
| 52:Y6:41:PRO:CG    | 52:Y6:45:LYS:H     | 2.05                     | 0.68              |
| 2:QB:126:GLU:HG2   | 2:QB:126:GLU:O     | 1.92                     | 0.68              |
| 2:QB:165:VAL:HG23  | 2:QB:166:ASP:H     | 1.57                     | 0.68              |
| 11:QK:124:LYS:HB3  | 11:QK:125:PHE:HD1  | 1.58                     | 0.68              |
| 20:QT:97:ALA:O     | 20:QT:99:LEU:N     | 2.27                     | 0.68              |
| 27:RD:17:THR:HG22  | 27:RD:205:VAL:N    | 2.08                     | 0.68              |
| 27:RD:122:ASP:CG   | 27:RD:123:ALA:H    | 2.00                     | 0.68              |
| 34:RO:8:LEU:HD22   | 34:RO:8:LEU:N      | 2.08                     | 0.68              |
| 35:RP:62:LEU:HD23  | 54:R8:25:MET:HB2   | 1.74                     | 0.68              |
| 52:R6:41:PRO:CG    | 52:R6:45:LYS:H     | 2.05                     | 0.68              |
| 4:XD:30:LYS:HA     | 4:XD:34:GLU:HB2    | 1.75                     | 0.68              |
| 7:XG:50:ILE:HB     | 7:XG:58:PRO:HB3    | 1.75                     | 0.68              |
| 13:XM:117:VAL:HG22 | 13:XM:118:ALA:H    | 1.59                     | 0.68              |
| 25:YA:1309:G:H4'   | 53:Y7:7:PRO:HB2    | 1.73                     | 0.68              |
| 3:QC:150:LYS:HB3   | 3:QC:201:TYR:HB2   | 1.75                     | 0.68              |
| 13:QM:90:LEU:CA    | 13:QM:93:ARG:HD2   | 2.23                     | 0.68              |
| 29:RF:185:ASP:HA   | 29:RF:188:ARG:CD   | 2.20                     | 0.68              |
| 50:R4:37:SER:C     | 50:R4:39:CYS:H     | 1.98                     | 0.68              |
| 52:R6:7:ILE:HG13   | 52:R6:8:LYS:N      | 2.06                     | 0.68              |
| 2:XB:126:GLU:HG2   | 2:XB:126:GLU:O     | 1.92                     | 0.68              |
| 10:XJ:75:ILE:HG13  | 10:XJ:76:ASN:N     | 2.05                     | 0.68              |
| 39:YT:11:GLU:CD    | 39:YT:11:GLU:N     | 2.47                     | 0.68              |
| 39:YT:111:ARG:C    | 39:YT:113:LYS:H    | 2.01                     | 0.68              |
| 44:YY:29:GLU:HB3   | 44:YY:38:ILE:HG12  | 1.74                     | 0.68              |
| 44:YY:61:ILE:CG2   | 44:YY:62:GLU:N     | 2.57                     | 0.68              |
| 1:QA:1305:G:H5'    | 21:QU:4:GLY:HA3    | 1.75                     | 0.68              |
| 2:QB:24:TRP:H      | 2:QB:24:TRP:CD1    | 2.11                     | 0.68              |
| 9:QI:28:VAL:HG13   | 9:QI:63:ILE:CG2    | 2.24                     | 0.68              |
| 14:QN:26:ARG:NH1   | 14:QN:43:CYS:SG    | 2.67                     | 0.68              |
| 20:QT:89:ARG:NH2   | 20:QT:104:LEU:HD21 | 2.09                     | 0.68              |
| 30:RG:112:PRO:CB   | 50:R4:37:SER:HB2   | 2.22                     | 0.68              |
| 33:RN:134:ARG:N    | 33:RN:135:PRO:HD3  | 1.97                     | 0.68              |
| 35:RP:26:GLY:O     | 35:RP:28:GLY:N     | 2.27                     | 0.68              |
| 47:R1:83:GLU:HG2   | 47:R1:84:GLY:N     | 2.09                     | 0.68              |
| 8:XH:112:LEU:HA    | 8:XH:134:ILE:HG12  | 1.75                     | 0.68              |
| 13:XM:78:ILE:HG23  | 13:XM:92:HIS:ND1   | 2.09                     | 0.68              |
| 25:YA:2312:U:OP1   | 30:YG:74:LYS:N     | 2.21                     | 0.68              |
| 31:YH:126:PRO:CD   | 31:YH:127:GLU:H    | 2.07                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:YS:100:ALA:HA  | 38:YS:103:GLU:HG2 | 1.75                     | 0.68              |
| 39:YT:109:GLU:O   | 39:YT:113:LYS:HB2 | 1.94                     | 0.68              |
| 44:YY:2:ARG:HH11  | 44:YY:2:ARG:HG2   | 1.57                     | 0.68              |
| 4:QD:198:VAL:HG12 | 4:QD:199:ASN:N    | 2.09                     | 0.68              |
| 14:QN:6:LEU:O     | 14:QN:6:LEU:HD23  | 1.93                     | 0.68              |
| 25:RA:1858:G:O2'  | 25:RA:1884:A:N6   | 2.26                     | 0.68              |
| 31:RH:126:PRO:HB2 | 31:RH:130:ARG:O   | 1.93                     | 0.68              |
| 34:RO:25:LEU:HB2  | 34:RO:38:VAL:HG13 | 1.74                     | 0.68              |
| 39:RT:109:GLU:O   | 39:RT:113:LYS:HB2 | 1.94                     | 0.68              |
| 44:RY:40:GLU:HA   | 44:RY:64:GLU:OE1  | 1.94                     | 0.68              |
| 50:R4:15:ILE:N    | 50:R4:15:ILE:HD13 | 2.09                     | 0.68              |
| 8:XH:6:ILE:HD12   | 8:XH:6:ILE:N      | 2.08                     | 0.68              |
| 25:YA:2789:C:H1'  | 25:YA:2892:A:H2   | 1.58                     | 0.68              |
| 30:YG:171:ALA:O   | 30:YG:175:LEU:HG  | 1.93                     | 0.68              |
| 31:YH:4:ILE:HG13  | 31:YH:6:ARG:NE    | 2.08                     | 0.68              |
| 31:YH:126:PRO:HB2 | 31:YH:130:ARG:O   | 1.93                     | 0.68              |
| 33:YN:46:VAL:O    | 33:YN:47:ALA:HB3  | 1.92                     | 0.68              |
| 36:YQ:80:GLU:HG3  | 36:YQ:81:VAL:H    | 1.58                     | 0.68              |
| 39:YT:50:ILE:HG22 | 39:YT:62:THR:OG1  | 1.94                     | 0.68              |
| 41:YV:18:LEU:O    | 41:YV:95:LEU:HA   | 1.94                     | 0.68              |
| 44:YY:40:GLU:HA   | 44:YY:64:GLU:OE1  | 1.93                     | 0.68              |
| 47:Y1:4:VAL:HG23  | 47:Y1:10:LYS:O    | 1.92                     | 0.68              |
| 48:Y2:23:LYS:O    | 48:Y2:27:GLU:OE1  | 2.11                     | 0.68              |
| 25:RA:1187:G:H5'' | 41:RV:81:TYR:CE2  | 2.28                     | 0.68              |
| 25:RA:1980:G:O2'  | 25:RA:1982:C:OP2  | 2.10                     | 0.68              |
| 25:RA:2298:A:H62  | 25:RA:2318:G:H8   | 1.42                     | 0.68              |
| 25:RA:2784:C:H5'' | 28:RE:41:LYS:NZ   | 2.09                     | 0.68              |
| 27:RD:17:THR:CG2  | 27:RD:204:ILE:HA  | 2.23                     | 0.68              |
| 31:RH:88:LEU:H    | 31:RH:88:LEU:HD22 | 1.58                     | 0.68              |
| 31:RH:126:PRO:HG2 | 31:RH:127:GLU:H   | 1.59                     | 0.68              |
| 36:RQ:12:GLN:CG   | 36:RQ:73:PRO:HD2  | 2.21                     | 0.68              |
| 37:RR:29:LEU:HD23 | 37:RR:79:LEU:HD12 | 1.75                     | 0.68              |
| 38:RS:100:ALA:HA  | 38:RS:103:GLU:HG2 | 1.75                     | 0.68              |
| 39:RT:108:ARG:HA  | 39:RT:111:ARG:CZ  | 2.23                     | 0.68              |
| 41:RV:18:LEU:O    | 41:RV:95:LEU:HA   | 1.94                     | 0.68              |
| 47:R1:64:ALA:HA   | 47:R1:67:ILE:HG13 | 1.75                     | 0.68              |
| 1:XA:191:G:C4     | 20:XT:105:SER:HB3 | 2.28                     | 0.68              |
| 4:XD:188:LEU:HD23 | 4:XD:189:PRO:HD2  | 1.75                     | 0.68              |
| 10:XJ:96:ILE:N    | 10:XJ:96:ILE:HD13 | 2.09                     | 0.68              |
| 17:XQ:59:ILE:HD13 | 17:XQ:59:ILE:N    | 2.09                     | 0.68              |
| 25:YA:10:G:N2     | 25:YA:2802:G:OP1  | 2.27                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:YE:9:VAL:HB    | 28:YE:25:VAL:HG23  | 1.76                     | 0.68              |
| 30:YG:112:PRO:CB  | 50:Y4:37:SER:HB2   | 2.22                     | 0.68              |
| 31:YH:4:ILE:HG13  | 31:YH:6:ARG:NH1    | 2.09                     | 0.68              |
| 42:YW:29:LEU:HD21 | 42:YW:33:ARG:NE    | 2.09                     | 0.68              |
| 1:QA:27:G:H4'     | 4:QD:209:ARG:HG3   | 1.75                     | 0.68              |
| 1:QA:411:A:H62    | 1:QA:413:G:H21     | 1.40                     | 0.68              |
| 2:QB:215:LEU:O    | 2:QB:219:VAL:HG23  | 1.94                     | 0.68              |
| 9:QI:48:GLU:N     | 9:QI:49:PRO:HD2    | 2.09                     | 0.68              |
| 36:RQ:88:GLY:C    | 36:RQ:90:VAL:N     | 2.47                     | 0.68              |
| 36:RQ:104:PHE:HE1 | 36:RQ:125:LEU:HD11 | 1.58                     | 0.68              |
| 39:RT:50:ILE:HG22 | 39:RT:62:THR:OG1   | 1.94                     | 0.68              |
| 43:RX:12:VAL:HG11 | 43:RX:27:THR:OG1   | 1.93                     | 0.68              |
| 43:RX:18:TYR:C    | 43:RX:20:GLY:H     | 2.02                     | 0.68              |
| 51:R5:20:ARG:HA   | 51:R5:23:HIS:ND1   | 2.09                     | 0.68              |
| 4:XD:198:VAL:HG12 | 4:XD:199:ASN:N     | 2.09                     | 0.68              |
| 5:XE:63:ARG:O     | 5:XE:66:MET:HE2    | 1.94                     | 0.68              |
| 11:XK:124:LYS:HB3 | 11:XK:125:PHE:HD1  | 1.58                     | 0.68              |
| 21:XU:6:ARG:HE    | 21:XU:15:ARG:NE    | 1.91                     | 0.68              |
| 33:YN:131:GLN:CD  | 33:YN:132:ALA:H    | 2.01                     | 0.68              |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:H     | 1.58                     | 0.68              |
| 4:QD:96:LEU:HD22  | 4:QD:96:LEU:N      | 2.07                     | 0.68              |
| 10:QJ:81:THR:C    | 10:QJ:83:GLU:H     | 1.99                     | 0.68              |
| 25:RA:483:A:H4'   | 44:RY:49:VAL:HA    | 1.75                     | 0.68              |
| 29:RF:67:GLN:O    | 29:RF:67:GLN:CG    | 2.32                     | 0.68              |
| 38:RS:57:LYS:HD3  | 38:RS:57:LYS:H     | 1.58                     | 0.68              |
| 47:R1:20:ARG:HH11 | 47:R1:20:ARG:HG2   | 1.58                     | 0.68              |
| 1:XA:7:G:H5'      | 1:XA:298:A:O4'     | 1.94                     | 0.68              |
| 1:XA:1014:A:H4'   | 19:XS:14:HIS:CD2   | 2.29                     | 0.68              |
| 6:XF:3:ARG:HB3    | 6:XF:93:SER:HB2    | 1.75                     | 0.68              |
| 8:XH:20:TYR:HE2   | 8:XH:75:ARG:HD2    | 1.59                     | 0.68              |
| 13:XM:90:LEU:CA   | 13:XM:93:ARG:HD2   | 2.23                     | 0.68              |
| 13:XM:119:GLY:HA3 | 22:XV:29:G:OP1     | 1.93                     | 0.68              |
| 27:YD:241:PRO:O   | 27:YD:243:GLY:N    | 2.27                     | 0.68              |
| 28:YE:16:ARG:O    | 28:YE:16:ARG:HG3   | 1.93                     | 0.68              |
| 33:YN:96:GLU:CG   | 33:YN:97:ARG:H     | 2.00                     | 0.68              |
| 35:YP:39:LYS:CA   | 35:YP:45:LEU:HD11  | 2.23                     | 0.68              |
| 36:YQ:90:VAL:CG1  | 36:YQ:91:GLU:N     | 2.57                     | 0.68              |
| 36:YQ:133:ARG:O   | 36:YQ:134:ARG:HB2  | 1.94                     | 0.68              |
| 43:YX:18:TYR:C    | 43:YX:20:GLY:H     | 2.02                     | 0.68              |
| 47:Y1:74:VAL:HG12 | 47:Y1:74:VAL:O     | 1.93                     | 0.68              |
| 50:Y4:15:ILE:N    | 50:Y4:15:ILE:HD13  | 2.09                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:QE:53:LEU:HD12  | 5:QE:53:LEU:N      | 2.09                     | 0.68              |
| 15:QO:61:GLY:C    | 15:QO:65:ARG:HH12  | 2.02                     | 0.68              |
| 16:QP:66:PRO:HG2  | 16:QP:71:ARG:NH1   | 2.09                     | 0.68              |
| 17:QQ:59:ILE:HD13 | 17:QQ:59:ILE:N     | 2.09                     | 0.68              |
| 44:RY:49:VAL:O    | 44:RY:51:VAL:N     | 2.27                     | 0.68              |
| 45:RZ:70:LEU:HB2  | 45:RZ:91:LEU:HD21  | 1.76                     | 0.68              |
| 47:R1:87:PRO:O    | 47:R1:88:LYS:C     | 2.37                     | 0.68              |
| 2:XB:24:TRP:CD1   | 2:XB:24:TRP:H      | 2.11                     | 0.68              |
| 7:XG:79:ARG:NH2   | 7:XG:82:GLY:HA2    | 2.09                     | 0.68              |
| 10:XJ:6:ILE:HG22  | 10:XJ:98:ILE:CG1   | 2.16                     | 0.68              |
| 25:YA:1068:G:O2'  | 25:YA:1096:A:N3    | 2.26                     | 0.68              |
| 25:YA:1795:C:O2   | 27:YD:255:LYS:HE2  | 1.94                     | 0.68              |
| 25:YA:2777:G:OP2  | 25:YA:2781:A:O2'   | 2.12                     | 0.68              |
| 44:YY:21:LYS:HG3  | 44:YY:22:GLY:N     | 2.09                     | 0.68              |
| 47:Y1:20:ARG:HH11 | 47:Y1:20:ARG:HG2   | 1.58                     | 0.68              |
| 48:Y2:64:LEU:HD22 | 48:Y2:68:ARG:HD2   | 1.76                     | 0.68              |
| 2:QB:7:VAL:HG22   | 2:QB:8:LYS:HD3     | 1.76                     | 0.67              |
| 10:QJ:48:THR:HA   | 10:QJ:62:HIS:HB3   | 1.75                     | 0.67              |
| 25:RA:1012:U:O2'  | 25:RA:1013:C:OP2   | 2.11                     | 0.67              |
| 28:RE:13:ARG:HH11 | 28:RE:13:ARG:CB    | 2.07                     | 0.67              |
| 29:RF:184:TYR:O   | 29:RF:188:ARG:HG3  | 1.93                     | 0.67              |
| 36:RQ:90:VAL:CG1  | 36:RQ:91:GLU:N     | 2.57                     | 0.67              |
| 48:R2:40:SER:C    | 48:R2:42:GLY:H     | 2.00                     | 0.67              |
| 7:XG:138:LYS:HE2  | 7:XG:142:GLU:OE2   | 1.94                     | 0.67              |
| 31:YH:77:LYS:HG2  | 31:YH:77:LYS:O     | 1.94                     | 0.67              |
| 31:YH:126:PRO:HG2 | 31:YH:127:GLU:H    | 1.59                     | 0.67              |
| 39:YT:50:ILE:CD1  | 39:YT:102:ILE:HD11 | 2.24                     | 0.67              |
| 7:QG:79:ARG:NH2   | 7:QG:82:GLY:HA2    | 2.09                     | 0.67              |
| 8:QH:14:ARG:O     | 8:QH:18:ARG:HD3    | 1.94                     | 0.67              |
| 8:QH:100:ILE:HB   | 8:QH:125:ARG:NH1   | 2.09                     | 0.67              |
| 10:QJ:96:ILE:HD13 | 10:QJ:96:ILE:N     | 2.09                     | 0.67              |
| 17:QQ:74:LEU:HD12 | 17:QQ:75:ARG:HG2   | 1.76                     | 0.67              |
| 28:RE:116:VAL:O   | 28:RE:117:MET:HB3  | 1.94                     | 0.67              |
| 29:RF:107:LYS:O   | 29:RF:108:LYS:C    | 2.36                     | 0.67              |
| 36:RQ:133:ARG:O   | 36:RQ:134:ARG:HB2  | 1.94                     | 0.67              |
| 39:RT:111:ARG:C   | 39:RT:113:LYS:H    | 2.01                     | 0.67              |
| 52:R6:48:VAL:HG13 | 52:R6:49:HIS:H     | 1.59                     | 0.67              |
| 2:XB:165:VAL:HG23 | 2:XB:166:ASP:H     | 1.57                     | 0.67              |
| 3:XC:150:LYS:HB3  | 3:XC:201:TYR:HB2   | 1.75                     | 0.67              |
| 9:XI:48:GLU:N     | 9:XI:49:PRO:HD2    | 2.10                     | 0.67              |
| 13:XM:36:LYS:HD3  | 13:XM:36:LYS:C     | 2.20                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:265:A:N6    | 25:YA:427:U:O2'    | 2.28                     | 0.67              |
| 28:YE:116:VAL:O   | 28:YE:117:MET:HB3  | 1.94                     | 0.67              |
| 34:YO:14:THR:O    | 34:YO:51:ALA:HB3   | 1.95                     | 0.67              |
| 35:YP:65:ARG:HH11 | 35:YP:65:ARG:CG    | 2.06                     | 0.67              |
| 38:YS:35:ILE:HD13 | 38:YS:101:LEU:HD23 | 1.76                     | 0.67              |
| 1:QA:673:G:H2'    | 1:QA:674:G:C8      | 2.29                     | 0.67              |
| 4:QD:79:PHE:C     | 4:QD:79:PHE:CD2    | 2.71                     | 0.67              |
| 12:QL:10:LEU:HB3  | 17:QQ:32:TYR:CE2   | 2.30                     | 0.67              |
| 14:QN:25:VAL:CG2  | 14:QN:38:GLY:O     | 2.31                     | 0.67              |
| 31:RH:89:ILE:HG12 | 31:RH:89:ILE:O     | 1.92                     | 0.67              |
| 36:RQ:104:PHE:CE1 | 36:RQ:125:LEU:HD11 | 2.29                     | 0.67              |
| 2:XB:71:VAL:CG2   | 2:XB:164:VAL:HG22  | 2.25                     | 0.67              |
| 3:XC:147:LYS:O    | 3:XC:203:PHE:HB3   | 1.92                     | 0.67              |
| 4:XD:29:PRO:O     | 4:XD:30:LYS:HD3    | 1.94                     | 0.67              |
| 4:XD:120:LEU:HD22 | 4:XD:125:HIS:HB2   | 1.74                     | 0.67              |
| 9:XI:127:LYS:CE   | 22:XV:34:C:OP2     | 2.42                     | 0.67              |
| 36:YQ:12:GLN:CG   | 36:YQ:73:PRO:HD2   | 2.21                     | 0.67              |
| 36:YQ:33:GLY:HA2  | 36:YQ:105:GLU:HA   | 1.76                     | 0.67              |
| 4:QD:173:TRP:CD2  | 4:QD:189:PRO:HB3   | 2.30                     | 0.67              |
| 11:QK:95:ILE:HD12 | 11:QK:108:ILE:HD13 | 1.77                     | 0.67              |
| 27:RD:135:PHE:CD2 | 27:RD:135:PHE:N    | 2.62                     | 0.67              |
| 28:RE:14:ILE:HG12 | 28:RE:15:PHE:N     | 2.06                     | 0.67              |
| 37:RR:26:LYS:HE2  | 37:RR:70:LEU:O     | 1.95                     | 0.67              |
| 38:RS:35:ILE:HD13 | 38:RS:101:LEU:HD23 | 1.76                     | 0.67              |
| 41:RV:25:LEU:H    | 41:RV:92:THR:HG21  | 1.60                     | 0.67              |
| 1:XA:991:U:O4     | 1:XA:1212:U:O2'    | 2.12                     | 0.67              |
| 8:XH:14:ARG:O     | 8:XH:18:ARG:HD3    | 1.94                     | 0.67              |
| 9:XI:28:VAL:HG13  | 9:XI:63:ILE:CG2    | 2.24                     | 0.67              |
| 11:XK:95:ILE:HD12 | 11:XK:108:ILE:HD13 | 1.76                     | 0.67              |
| 20:XT:83:ARG:HA   | 20:XT:86:ARG:HD3   | 1.76                     | 0.67              |
| 25:YA:451:C:H4'   | 29:YF:52:LYS:NZ    | 2.09                     | 0.67              |
| 27:YD:44:ASN:N    | 27:YD:44:ASN:ND2   | 2.42                     | 0.67              |
| 34:YO:25:LEU:HB2  | 34:YO:38:VAL:HG13  | 1.74                     | 0.67              |
| 35:YP:26:GLY:O    | 35:YP:28:GLY:N     | 2.26                     | 0.67              |
| 36:YQ:90:VAL:O    | 36:YQ:92:GLY:N     | 2.25                     | 0.67              |
| 38:YS:26:LEU:HD12 | 38:YS:39:ILE:CD1   | 2.23                     | 0.67              |
| 39:YT:108:ARG:HA  | 39:YT:111:ARG:CZ   | 2.23                     | 0.67              |
| 44:YY:49:VAL:O    | 44:YY:51:VAL:N     | 2.27                     | 0.67              |
| 6:QF:67:MET:HB2   | 6:QF:68:PRO:HD2    | 1.75                     | 0.67              |
| 10:QJ:6:ILE:HG22  | 10:QJ:98:ILE:CG1   | 2.16                     | 0.67              |
| 13:QM:23:TYR:CB   | 13:QM:67:GLU:HG2   | 2.25                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:807:U:OP2   | 35:RP:41:ARG:NH1   | 2.28                     | 0.67              |
| 34:RO:13:ASN:ND2  | 34:RO:96:THR:O     | 2.28                     | 0.67              |
| 36:RQ:20:ALA:HB1  | 36:RQ:99:PRO:HD2   | 1.77                     | 0.67              |
| 40:RU:92:ARG:O    | 40:RU:94:ASN:N     | 2.25                     | 0.67              |
| 42:RW:29:LEU:HD21 | 42:RW:33:ARG:NE    | 2.08                     | 0.67              |
| 5:XE:78:HIS:HA    | 8:XH:105:ARG:HB2   | 1.76                     | 0.67              |
| 7:XG:120:ILE:O    | 7:XG:124:LEU:HB2   | 1.95                     | 0.67              |
| 9:XI:46:ALA:HA    | 9:XI:78:LYS:HB2    | 1.75                     | 0.67              |
| 16:XP:66:PRO:HG2  | 16:XP:71:ARG:NH1   | 2.09                     | 0.67              |
| 28:YE:13:ARG:HH11 | 28:YE:13:ARG:CB    | 2.07                     | 0.67              |
| 38:YS:67:ARG:HB2  | 38:YS:67:ARG:CZ    | 2.24                     | 0.67              |
| 44:YY:14:LEU:HD23 | 44:YY:15:VAL:N     | 2.10                     | 0.67              |
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21  | 1.76                     | 0.67              |
| 50:Y4:33:VAL:HG12 | 50:Y4:34:GLU:N     | 2.10                     | 0.67              |
| 2:QB:24:TRP:H     | 2:QB:24:TRP:HD1    | 1.43                     | 0.67              |
| 5:QE:63:ARG:O     | 5:QE:66:MET:HE2    | 1.94                     | 0.67              |
| 7:QG:50:ILE:HB    | 7:QG:58:PRO:HB3    | 1.75                     | 0.67              |
| 7:QG:140:ASP:C    | 7:QG:142:GLU:H     | 2.03                     | 0.67              |
| 25:RA:2198:A:O2'  | 25:RA:2199:A:O5'   | 2.13                     | 0.67              |
| 28:RE:10:GLY:H    | 28:RE:25:VAL:HG23  | 1.60                     | 0.67              |
| 42:RW:60:ASN:C    | 42:RW:61:ASN:HD22  | 2.03                     | 0.67              |
| 1:XA:1178:G:N2    | 1:XA:1181:G:N7     | 2.43                     | 0.67              |
| 3:XC:195:VAL:HG12 | 3:XC:196:LEU:N     | 2.07                     | 0.67              |
| 4:XD:29:PRO:C     | 4:XD:30:LYS:HD3    | 2.19                     | 0.67              |
| 16:XP:21:VAL:HG11 | 16:XP:59:TRP:CD1   | 2.30                     | 0.67              |
| 28:YE:26:ILE:HD13 | 28:YE:27:LEU:N     | 2.10                     | 0.67              |
| 29:YF:184:TYR:O   | 29:YF:188:ARG:HG3  | 1.94                     | 0.67              |
| 36:YQ:104:PHE:CE1 | 36:YQ:125:LEU:HD11 | 2.29                     | 0.67              |
| 38:YS:52:SER:O    | 38:YS:56:LEU:HD22  | 1.93                     | 0.67              |
| 51:Y5:4:HIS:HB3   | 51:Y5:5:PRO:HD3    | 1.75                     | 0.67              |
| 52:Y6:48:VAL:HG13 | 52:Y6:49:HIS:H     | 1.60                     | 0.67              |
| 6:QF:96:PRO:HB3   | 18:QR:30:ASP:OD2   | 1.95                     | 0.67              |
| 7:QG:28:ASN:O     | 7:QG:31:MET:HB3    | 1.95                     | 0.67              |
| 7:QG:120:ILE:O    | 7:QG:124:LEU:HB2   | 1.95                     | 0.67              |
| 13:QM:13:LYS:HA   | 13:QM:44:ARG:HD2   | 1.77                     | 0.67              |
| 13:QM:78:ILE:HG23 | 13:QM:92:HIS:ND1   | 2.09                     | 0.67              |
| 25:RA:530:G:O2'   | 25:RA:532:A:N7     | 2.27                     | 0.67              |
| 31:RH:4:ILE:HG13  | 31:RH:6:ARG:NH1    | 2.09                     | 0.67              |
| 31:RH:126:PRO:CD  | 31:RH:127:GLU:H    | 2.07                     | 0.67              |
| 44:RY:61:ILE:CG2  | 44:RY:62:GLU:N     | 2.56                     | 0.67              |
| 52:R6:43:CYS:SG   | 52:R6:44:ARG:HD3   | 2.35                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:136:C:H42    | 1:XA:227:G:H1      | 1.43                     | 0.67              |
| 10:XJ:54:PHE:CZ   | 10:XJ:55:LYS:NZ    | 2.61                     | 0.67              |
| 25:YA:482:A:H4'   | 44:YY:47:LYS:HD2   | 1.77                     | 0.67              |
| 25:YA:1169:G:H1   | 25:YA:1180:C:H42   | 1.41                     | 0.67              |
| 29:YF:107:LYS:O   | 29:YF:108:LYS:C    | 2.36                     | 0.67              |
| 40:YU:90:VAL:O    | 40:YU:92:ARG:N     | 2.26                     | 0.67              |
| 41:YV:25:LEU:H    | 41:YV:92:THR:HG21  | 1.60                     | 0.67              |
| 49:Y3:29:ARG:HB2  | 49:Y3:29:ARG:NH1   | 2.10                     | 0.67              |
| 51:Y5:20:ARG:HA   | 51:Y5:23:HIS:ND1   | 2.08                     | 0.67              |
| 9:QI:112:LYS:HA   | 9:QI:119:ALA:HB2   | 1.77                     | 0.67              |
| 13:QM:3:ARG:HD2   | 13:QM:9:ILE:HG12   | 1.77                     | 0.67              |
| 18:QR:70:ILE:O    | 18:QR:74:ARG:HG3   | 1.95                     | 0.67              |
| 19:QS:31:ILE:HG23 | 19:QS:49:ILE:HA    | 1.75                     | 0.67              |
| 25:RA:2420:C:H41  | 54:R8:30:ARG:HD2   | 1.60                     | 0.67              |
| 25:RA:2746:U:H5'' | 31:RH:138:LYS:HE2  | 1.77                     | 0.67              |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:HD2  | 1.77                     | 0.67              |
| 35:RP:90:ARG:NE   | 35:RP:91:PHE:HD1   | 1.93                     | 0.67              |
| 36:RQ:32:TYR:HD1  | 36:RQ:133:ARG:HA   | 1.60                     | 0.67              |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:H     | 1.57                     | 0.67              |
| 38:RS:107:GLU:H   | 38:RS:110:LEU:HD11 | 1.60                     | 0.67              |
| 45:RZ:72:ARG:NH2  | 45:RZ:97:GLU:O     | 2.28                     | 0.67              |
| 50:R4:33:VAL:HG12 | 50:R4:34:GLU:N     | 2.10                     | 0.67              |
| 2:XB:164:VAL:HB   | 2:XB:186:ALA:CB    | 2.25                     | 0.67              |
| 4:XD:11:LEU:CD2   | 4:XD:66:ARG:HD3    | 2.17                     | 0.67              |
| 9:XI:33:PHE:CZ    | 9:XI:47:LEU:HD21   | 2.30                     | 0.67              |
| 50:Y4:16:CYS:SG   | 50:Y4:33:VAL:HB    | 2.35                     | 0.67              |
| 4:QD:52:SER:HB3   | 4:QD:55:ALA:HB2    | 1.77                     | 0.67              |
| 7:QG:138:LYS:HE2  | 7:QG:142:GLU:OE2   | 1.94                     | 0.67              |
| 8:QH:10:LEU:HD23  | 8:QH:10:LEU:H      | 1.59                     | 0.67              |
| 20:QT:83:ARG:HA   | 20:QT:86:ARG:HD3   | 1.76                     | 0.67              |
| 28:RE:16:ARG:O    | 28:RE:16:ARG:HG3   | 1.93                     | 0.67              |
| 31:RH:125:VAL:CG1 | 31:RH:126:PRO:HG3  | 2.25                     | 0.67              |
| 36:RQ:90:VAL:O    | 36:RQ:92:GLY:N     | 2.25                     | 0.67              |
| 48:R2:47:ASN:H    | 48:R2:47:ASN:ND2   | 1.92                     | 0.67              |
| 4:XD:173:TRP:CD2  | 4:XD:189:PRO:HB3   | 2.30                     | 0.67              |
| 7:XG:28:ASN:O     | 7:XG:31:MET:HB3    | 1.95                     | 0.67              |
| 17:XQ:56:VAL:HB   | 17:XQ:78:GLU:HB3   | 1.76                     | 0.67              |
| 27:YD:35:LYS:CA   | 27:YD:64:ILE:HG22  | 2.25                     | 0.67              |
| 28:YE:62:PRO:O    | 28:YE:64:LYS:N     | 2.28                     | 0.67              |
| 29:YF:34:TRP:HA   | 35:YP:6:LEU:HD12   | 1.77                     | 0.67              |
| 31:YH:88:LEU:H    | 31:YH:88:LEU:HD22  | 1.59                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:YV:44:LYS:O    | 41:YV:46:VAL:N     | 2.28                     | 0.67              |
| 1:QA:642:A:N3     | 8:QH:113:SER:OG    | 2.26                     | 0.67              |
| 9:QI:33:PHE:CZ    | 9:QI:47:LEU:HD21   | 2.30                     | 0.67              |
| 20:QT:36:LEU:HD12 | 20:QT:55:ILE:HG23  | 1.76                     | 0.67              |
| 25:RA:1286:A:O2'  | 25:RA:1288:U:OP2   | 2.13                     | 0.67              |
| 25:RA:2344:U:OP1  | 52:R6:38:LYS:HD3   | 1.94                     | 0.67              |
| 27:RD:35:LYS:CG   | 27:RD:64:ILE:N     | 2.56                     | 0.67              |
| 27:RD:241:PRO:O   | 27:RD:243:GLY:N    | 2.28                     | 0.67              |
| 35:RP:122:PRO:HA  | 35:RP:141:ALA:O    | 1.95                     | 0.67              |
| 15:XO:61:GLY:C    | 15:XO:65:ARG:HH12  | 2.02                     | 0.67              |
| 33:YN:57:ALA:HA   | 33:YN:60:ILE:HD11  | 1.77                     | 0.67              |
| 34:YO:13:ASN:ND2  | 34:YO:96:THR:O     | 2.28                     | 0.67              |
| 35:YP:61:ARG:H    | 35:YP:61:ARG:CD    | 2.08                     | 0.67              |
| 41:YV:53:GLU:HG2  | 41:YV:53:GLU:O     | 1.94                     | 0.67              |
| 47:Y1:83:GLU:HG2  | 47:Y1:84:GLY:N     | 2.09                     | 0.67              |
| 47:Y1:86:SER:N    | 47:Y1:87:PRO:HD2   | 2.10                     | 0.67              |
| 1:QA:527:G:O6     | 12:QL:49:ASN:ND2   | 2.23                     | 0.66              |
| 2:QB:164:VAL:HB   | 2:QB:186:ALA:CB    | 2.25                     | 0.66              |
| 25:RA:498:G:N3    | 44:RY:47:LYS:NZ    | 2.41                     | 0.66              |
| 28:RE:36:ARG:HH11 | 28:RE:36:ARG:HB3   | 1.60                     | 0.66              |
| 31:RH:77:LYS:HG2  | 31:RH:77:LYS:O     | 1.94                     | 0.66              |
| 43:RX:57:LEU:HD12 | 43:RX:78:LYS:HB2   | 1.77                     | 0.66              |
| 44:RY:21:LYS:HG3  | 44:RY:22:GLY:N     | 2.09                     | 0.66              |
| 49:R3:29:ARG:HB2  | 49:R3:29:ARG:NH1   | 2.10                     | 0.66              |
| 1:XA:527:G:O6     | 12:XL:49:ASN:ND2   | 2.29                     | 0.66              |
| 3:XC:73:PRO:O     | 3:XC:76:VAL:HG22   | 1.95                     | 0.66              |
| 25:YA:84:A:N1     | 25:YA:98:G:O2'     | 2.24                     | 0.66              |
| 25:YA:674:G:C1'   | 29:YF:74:ARG:HD3   | 2.24                     | 0.66              |
| 29:YF:46:ARG:HH11 | 29:YF:46:ARG:CG    | 2.04                     | 0.66              |
| 36:YQ:104:PHE:HE1 | 36:YQ:125:LEU:HD11 | 1.59                     | 0.66              |
| 44:YY:60:PHE:O    | 44:YY:61:ILE:HD12  | 1.95                     | 0.66              |
| 47:Y1:87:PRO:O    | 47:Y1:88:LYS:C     | 2.37                     | 0.66              |
| 52:Y6:43:CYS:SG   | 52:Y6:44:ARG:HD3   | 2.35                     | 0.66              |
| 1:QA:973:G:H3'    | 1:QA:974:A:H5''    | 1.76                     | 0.66              |
| 1:QA:1312:G:H5''  | 50:R4:67:TYR:OH    | 1.95                     | 0.66              |
| 2:QB:71:VAL:CG2   | 2:QB:164:VAL:HG22  | 2.25                     | 0.66              |
| 8:QH:20:TYR:HE2   | 8:QH:75:ARG:HD2    | 1.60                     | 0.66              |
| 25:RA:155:C:H42   | 25:RA:171:G:H1     | 1.41                     | 0.66              |
| 35:RP:66:GLY:O    | 35:RP:67:MET:HB3   | 1.94                     | 0.66              |
| 44:RY:42:VAL:CG1  | 44:RY:65:ALA:HB3   | 2.25                     | 0.66              |
| 47:R1:80:LEU:HD23 | 47:R1:80:LEU:N     | 2.10                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:6:ILE:HD11   | 10:XJ:72:VAL:CB    | 2.24                     | 0.66              |
| 10:XJ:34:VAL:HG22  | 10:XJ:74:ILE:HG22  | 1.77                     | 0.66              |
| 29:YF:103:LYS:HA   | 29:YF:106:ARG:CG   | 2.21                     | 0.66              |
| 35:YP:122:PRO:HA   | 35:YP:141:ALA:O    | 1.95                     | 0.66              |
| 42:YW:18:ARG:HG3   | 42:YW:76:VAL:HG13  | 1.77                     | 0.66              |
| 42:YW:60:ASN:C     | 42:YW:61:ASN:HD22  | 2.03                     | 0.66              |
| 47:Y1:56:GLN:N     | 47:Y1:56:GLN:HE21  | 1.93                     | 0.66              |
| 4:QD:196:LEU:C     | 4:QD:198:VAL:H     | 2.03                     | 0.66              |
| 8:QH:6:ILE:H       | 8:QH:6:ILE:CD1     | 2.07                     | 0.66              |
| 25:RA:1026:U:H4'   | 25:RA:1027:A:OP1   | 1.96                     | 0.66              |
| 25:RA:2562:U:O2'   | 34:RO:23:ARG:NH1   | 2.28                     | 0.66              |
| 25:RA:2723:C:O3'   | 37:RR:1:MET:HE3    | 1.95                     | 0.66              |
| 27:RD:80:ALA:HB3   | 27:RD:94:LEU:CD1   | 2.26                     | 0.66              |
| 29:RF:34:TRP:HA    | 35:RP:6:LEU:HD12   | 1.77                     | 0.66              |
| 34:RO:86:ILE:H     | 34:RO:86:ILE:HD12  | 1.60                     | 0.66              |
| 38:RS:67:ARG:HB2   | 38:RS:67:ARG:CZ    | 2.24                     | 0.66              |
| 2:XB:215:LEU:O     | 2:XB:219:VAL:HG23  | 1.94                     | 0.66              |
| 4:XD:14:ARG:O      | 4:XD:14:ARG:HD3    | 1.95                     | 0.66              |
| 8:XH:29:SER:HB3    | 8:XH:32:LYS:CG     | 2.22                     | 0.66              |
| 8:XH:100:ILE:HB    | 8:XH:125:ARG:NH1   | 2.09                     | 0.66              |
| 14:XN:32:SER:O     | 14:XN:40:CYS:C     | 2.37                     | 0.66              |
| 20:XT:89:ARG:NH2   | 20:XT:104:LEU:HD21 | 2.09                     | 0.66              |
| 28:YE:51:PHE:O     | 28:YE:52:LEU:C     | 2.38                     | 0.66              |
| 30:YG:179:PRO:HG3  | 50:Y4:38:LYS:HZ2   | 1.59                     | 0.66              |
| 33:YN:58:ASP:H     | 33:YN:60:ILE:CD1   | 2.09                     | 0.66              |
| 36:YQ:32:TYR:HD1   | 36:YQ:133:ARG:HA   | 1.60                     | 0.66              |
| 44:YY:75:ILE:HG12  | 44:YY:76:CYS:N     | 2.10                     | 0.66              |
| 48:Y2:65:ASN:HB3   | 48:Y2:69:ARG:NH1   | 2.10                     | 0.66              |
| 3:QC:73:PRO:O      | 3:QC:76:VAL:HG22   | 1.95                     | 0.66              |
| 13:QM:117:VAL:HG22 | 13:QM:118:ALA:H    | 1.59                     | 0.66              |
| 16:QP:21:VAL:HG11  | 16:QP:59:TRP:CD1   | 2.30                     | 0.66              |
| 27:RD:145:VAL:HG12 | 27:RD:146:GLU:O    | 1.96                     | 0.66              |
| 35:RP:1:MET:CE     | 35:RP:5:ASP:HB3    | 2.24                     | 0.66              |
| 3:XC:140:ARG:CZ    | 3:XC:140:ARG:HB2   | 2.25                     | 0.66              |
| 4:XD:52:SER:O      | 4:XD:56:VAL:HG23   | 1.95                     | 0.66              |
| 4:XD:79:PHE:C      | 4:XD:79:PHE:CD2    | 2.71                     | 0.66              |
| 18:XR:70:ILE:O     | 18:XR:74:ARG:HG3   | 1.95                     | 0.66              |
| 28:YE:28:ALA:O     | 28:YE:93:VAL:HG23  | 1.96                     | 0.66              |
| 38:YS:106:ARG:HA   | 38:YS:110:LEU:CD2  | 2.25                     | 0.66              |
| 51:Y5:56:LYS:H     | 51:Y5:56:LYS:CD    | 2.07                     | 0.66              |
| 1:QA:78:G:O6       | 1:QA:91:C:N4       | 2.28                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:QE:75:THR:HG23  | 5:QE:76:ILE:N      | 2.11                     | 0.66              |
| 19:QS:65:ASN:N    | 19:QS:65:ASN:HD22  | 1.94                     | 0.66              |
| 25:RA:1000:A:OP2  | 25:RA:1154:G:N1    | 2.19                     | 0.66              |
| 31:RH:168:PRO:O   | 31:RH:169:VAL:HG12 | 1.96                     | 0.66              |
| 34:RO:14:THR:O    | 34:RO:51:ALA:HB3   | 1.95                     | 0.66              |
| 36:RQ:86:GLY:C    | 36:RQ:88:GLY:H     | 2.03                     | 0.66              |
| 41:RV:44:LYS:O    | 41:RV:46:VAL:N     | 2.28                     | 0.66              |
| 44:RY:94:LYS:HE3  | 44:RY:101:LYS:NZ   | 2.11                     | 0.66              |
| 7:XG:69:VAL:HG12  | 7:XG:69:VAL:O      | 1.95                     | 0.66              |
| 8:XH:84:ARG:HG3   | 8:XH:84:ARG:NH1    | 2.10                     | 0.66              |
| 27:YD:172:TYR:HB3 | 27:YD:184:LYS:HG2  | 1.77                     | 0.66              |
| 36:YQ:88:GLY:C    | 36:YQ:90:VAL:H     | 2.02                     | 0.66              |
| 40:YU:88:ILE:HD13 | 40:YU:88:ILE:N     | 2.10                     | 0.66              |
| 47:Y1:73:LEU:C    | 47:Y1:75:GLU:H     | 2.03                     | 0.66              |
| 48:Y2:47:ASN:H    | 48:Y2:47:ASN:ND2   | 1.92                     | 0.66              |
| 51:Y5:40:LYS:NZ   | 51:Y5:48:GLU:HB2   | 2.10                     | 0.66              |
| 2:QB:25:ASN:O     | 2:QB:27:LYS:N      | 2.28                     | 0.66              |
| 2:QB:87:ARG:HH11  | 2:QB:223:ILE:CD1   | 2.09                     | 0.66              |
| 3:QC:101:LEU:HD23 | 3:QC:102:ASN:N     | 2.11                     | 0.66              |
| 6:QF:1:MET:HE1    | 6:QF:68:PRO:HB3    | 1.78                     | 0.66              |
| 7:QG:78:ARG:NH1   | 7:QG:80:VAL:HG23   | 2.11                     | 0.66              |
| 14:QN:40:CYS:SG   | 14:QN:43:CYS:N     | 2.67                     | 0.66              |
| 25:RA:210:C:OP2   | 53:R7:29:LYS:NZ    | 2.29                     | 0.66              |
| 27:RD:44:ASN:HB3  | 27:RD:49:ILE:HG22  | 1.78                     | 0.66              |
| 28:RE:9:VAL:HB    | 28:RE:25:VAL:HG23  | 1.75                     | 0.66              |
| 30:RG:136:ARG:O   | 30:RG:154:GLY:HA3  | 1.95                     | 0.66              |
| 35:RP:81:GLN:NE2  | 35:RP:106:LEU:O    | 2.29                     | 0.66              |
| 36:RQ:33:GLY:HA2  | 36:RQ:105:GLU:HA   | 1.76                     | 0.66              |
| 40:RU:88:ILE:HD13 | 40:RU:88:ILE:N     | 2.10                     | 0.66              |
| 47:R1:51:VAL:HG11 | 47:R1:74:VAL:HG21  | 1.75                     | 0.66              |
| 47:R1:86:SER:N    | 47:R1:87:PRO:HD2   | 2.10                     | 0.66              |
| 13:XM:3:ARG:HD2   | 13:XM:9:ILE:HG12   | 1.77                     | 0.66              |
| 20:XT:97:ALA:O    | 20:XT:99:LEU:N     | 2.27                     | 0.66              |
| 25:YA:2311:A:C8   | 30:YG:82:LEU:HD11  | 2.31                     | 0.66              |
| 25:YA:2711:A:H5'' | 25:YA:2712:U:H5'   | 1.78                     | 0.66              |
| 30:YG:136:ARG:O   | 30:YG:154:GLY:HA3  | 1.95                     | 0.66              |
| 35:YP:66:GLY:O    | 35:YP:67:MET:HB3   | 1.94                     | 0.66              |
| 43:YX:11:PRO:HB3  | 43:YX:92:LEU:HD21  | 1.78                     | 0.66              |
| 54:Y8:30:ARG:O    | 54:Y8:31:HIS:HB2   | 1.96                     | 0.66              |
| 8:QH:23:SER:HA    | 8:QH:63:LEU:CD2    | 2.24                     | 0.66              |
| 13:QM:81:LEU:O    | 13:QM:84:ILE:HG22  | 1.95                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:QO:26:GLU:CD   | 15:QO:77:ARG:HH12  | 2.03                     | 0.66              |
| 25:RA:674:G:C1'   | 29:RF:74:ARG:HD3   | 2.26                     | 0.66              |
| 25:RA:900:A:H3'   | 25:RA:901:A:H8     | 1.60                     | 0.66              |
| 25:RA:1820:U:C2   | 27:RD:202:LYS:HB3  | 2.31                     | 0.66              |
| 27:RD:68:LYS:HB2  | 27:RD:70:TRP:CZ3   | 2.31                     | 0.66              |
| 28:RE:26:ILE:HD13 | 28:RE:27:LEU:N     | 2.10                     | 0.66              |
| 28:RE:101:ARG:CZ  | 28:RE:171:GLU:HB2  | 2.25                     | 0.66              |
| 38:RS:88:ASP:OD2  | 38:RS:90:GLY:N     | 2.28                     | 0.66              |
| 39:RT:50:ILE:CD1  | 39:RT:102:ILE:HD11 | 2.25                     | 0.66              |
| 44:RY:47:LYS:HG2  | 44:RY:60:PHE:CE1   | 2.31                     | 0.66              |
| 44:RY:75:ILE:HG12 | 44:RY:76:CYS:N     | 2.10                     | 0.66              |
| 13:XM:81:LEU:O    | 13:XM:84:ILE:HG22  | 1.95                     | 0.66              |
| 25:YA:1754:C:OP1  | 39:YT:96:ARG:NH1   | 2.23                     | 0.66              |
| 27:YD:135:PHE:CD2 | 27:YD:135:PHE:N    | 2.62                     | 0.66              |
| 35:YP:61:ARG:NH2  | 54:Y8:13:ARG:HD2   | 2.10                     | 0.66              |
| 36:YQ:20:ALA:HB1  | 36:YQ:99:PRO:HD2   | 1.77                     | 0.66              |
| 40:YU:65:ILE:HG12 | 40:YU:96:ALA:CB    | 2.26                     | 0.66              |
| 12:QL:126:LYS:C   | 12:QL:128:ALA:H    | 2.03                     | 0.66              |
| 25:RA:414:C:O2    | 25:RA:1864:U:O2'   | 2.14                     | 0.66              |
| 25:RA:1930:G:H2'  | 25:RA:1968:G:H1    | 1.59                     | 0.66              |
| 27:RD:35:LYS:CA   | 27:RD:64:ILE:HG22  | 2.26                     | 0.66              |
| 28:RE:62:PRO:O    | 28:RE:64:LYS:N     | 2.28                     | 0.66              |
| 29:RF:175:THR:O   | 29:RF:176:LEU:HB2  | 1.96                     | 0.66              |
| 33:RN:58:ASP:H    | 33:RN:60:ILE:CD1   | 2.08                     | 0.66              |
| 44:RY:14:LEU:HD23 | 44:RY:15:VAL:N     | 2.10                     | 0.66              |
| 2:XB:24:TRP:H     | 2:XB:24:TRP:HD1    | 1.43                     | 0.66              |
| 4:XD:196:LEU:C    | 4:XD:198:VAL:H     | 2.02                     | 0.66              |
| 12:XL:48:PRO:CD   | 12:XL:49:ASN:N     | 2.57                     | 0.66              |
| 13:XM:74:VAL:O    | 13:XM:78:ILE:HG13  | 1.96                     | 0.66              |
| 19:XS:35:SER:O    | 19:XS:71:LEU:HD12  | 1.96                     | 0.66              |
| 27:YD:68:LYS:HB2  | 27:YD:70:TRP:CZ3   | 2.31                     | 0.66              |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:CE1  | 2.29                     | 0.66              |
| 31:YH:125:VAL:CG1 | 31:YH:126:PRO:HG3  | 2.25                     | 0.66              |
| 34:YO:110:GLY:HA2 | 34:YO:112:MET:HE3  | 1.77                     | 0.66              |
| 35:YP:81:GLN:NE2  | 35:YP:106:LEU:O    | 2.29                     | 0.66              |
| 47:Y1:11:ARG:HB3  | 47:Y1:11:ARG:HH11  | 1.61                     | 0.66              |
| 17:QQ:56:VAL:HB   | 17:QQ:78:GLU:HB3   | 1.76                     | 0.66              |
| 27:RD:121:PRO:HB3 | 27:RD:135:PHE:CE1  | 2.29                     | 0.66              |
| 35:RP:61:ARG:NH2  | 54:R8:13:ARG:HD2   | 2.10                     | 0.66              |
| 50:R4:16:CYS:SG   | 50:R4:33:VAL:HB    | 2.35                     | 0.66              |
| 54:R8:30:ARG:O    | 54:R8:31:HIS:HB2   | 1.96                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:XE:75:THR:HG23   | 5:XE:76:ILE:N      | 2.11                     | 0.66              |
| 15:XO:26:GLU:CD    | 15:XO:77:ARG:HH12  | 2.03                     | 0.66              |
| 19:XS:15:LEU:O     | 19:XS:19:VAL:N     | 2.26                     | 0.66              |
| 30:YG:145:THR:HG23 | 50:Y4:28:LYS:NZ    | 2.11                     | 0.66              |
| 38:YS:88:ASP:OD2   | 38:YS:90:GLY:N     | 2.28                     | 0.66              |
| 38:YS:107:GLU:H    | 38:YS:110:LEU:HD11 | 1.60                     | 0.66              |
| 2:QB:87:ARG:O      | 2:QB:87:ARG:HD2    | 1.95                     | 0.66              |
| 7:QG:141:VAL:O     | 7:QG:141:VAL:HG12  | 1.95                     | 0.66              |
| 15:QO:25:THR:HG21  | 15:QO:70:LEU:HB2   | 1.77                     | 0.66              |
| 17:QQ:27:PHE:CZ    | 17:QQ:36:ILE:HD11  | 2.31                     | 0.66              |
| 25:RA:2364:C:OP1   | 46:R0:55:ARG:NH1   | 2.29                     | 0.66              |
| 27:RD:183:ARG:HH11 | 27:RD:183:ARG:CG   | 2.07                     | 0.66              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:CD2  | 2.26                     | 0.66              |
| 4:XD:52:SER:HB3    | 4:XD:55:ALA:HB2    | 1.77                     | 0.66              |
| 12:XL:26:ALA:O     | 12:XL:27:LEU:O     | 2.14                     | 0.66              |
| 27:YD:35:LYS:HE3   | 27:YD:64:ILE:C     | 2.21                     | 0.66              |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:CG   | 2.07                     | 0.66              |
| 28:YE:37:ARG:NE    | 28:YE:37:ARG:HA    | 2.11                     | 0.66              |
| 31:YH:124:GLU:HB3  | 31:YH:132:ARG:HD2  | 1.77                     | 0.66              |
| 33:YN:134:ARG:N    | 33:YN:135:PRO:HD3  | 1.97                     | 0.66              |
| 44:YY:94:LYS:HE3   | 44:YY:101:LYS:NZ   | 2.11                     | 0.66              |
| 47:Y1:80:LEU:HD23  | 47:Y1:80:LEU:N     | 2.10                     | 0.66              |
| 6:QF:41:GLU:O      | 6:QF:43:LEU:HD12   | 1.96                     | 0.65              |
| 7:QG:69:VAL:O      | 7:QG:69:VAL:HG12   | 1.95                     | 0.65              |
| 10:QJ:99:LYS:O     | 10:QJ:100:THR:HG23 | 1.96                     | 0.65              |
| 13:QM:36:LYS:HD3   | 13:QM:36:LYS:C     | 2.20                     | 0.65              |
| 25:RA:1251:C:OP1   | 40:RU:10:ARG:HG3   | 1.96                     | 0.65              |
| 25:RA:1398:C:OP1   | 43:RX:53:LYS:NZ    | 2.28                     | 0.65              |
| 25:RA:2287:A:N6    | 25:RA:2344:U:H3    | 1.94                     | 0.65              |
| 26:RB:52:A:H62     | 38:RS:33:LYS:HG3   | 1.62                     | 0.65              |
| 39:RT:22:PHE:CD2   | 39:RT:22:PHE:N     | 2.63                     | 0.65              |
| 41:RV:53:GLU:HG2   | 41:RV:53:GLU:O     | 1.94                     | 0.65              |
| 44:RY:99:CYS:SG    | 44:RY:100:ALA:N    | 2.69                     | 0.65              |
| 48:R2:64:LEU:HD22  | 48:R2:68:ARG:HD2   | 1.76                     | 0.65              |
| 7:XG:78:ARG:NH1    | 7:XG:80:VAL:HG23   | 2.11                     | 0.65              |
| 8:XH:10:LEU:HD23   | 8:XH:10:LEU:H      | 1.60                     | 0.65              |
| 10:XJ:39:PRO:HB3   | 10:XJ:70:ARG:HH12  | 1.61                     | 0.65              |
| 17:XQ:27:PHE:CZ    | 17:XQ:36:ILE:HD11  | 2.31                     | 0.65              |
| 28:YE:36:ARG:HH11  | 28:YE:36:ARG:HB3   | 1.60                     | 0.65              |
| 34:YO:113:LYS:O    | 34:YO:117:LEU:HD12 | 1.96                     | 0.65              |
| 42:YW:65:LEU:HD12  | 42:YW:68:ARG:NH1   | 2.10                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:YX:65:ARG:HD3   | 43:YX:65:ARG:N     | 2.11                     | 0.65              |
| 44:YY:35:TYR:CE1   | 44:YY:69:ALA:HB3   | 2.31                     | 0.65              |
| 44:YY:47:LYS:HG2   | 44:YY:60:PHE:CE1   | 2.31                     | 0.65              |
| 1:QA:523:A:H61     | 12:QL:92:ASP:HB2   | 1.61                     | 0.65              |
| 3:QC:140:ARG:CZ    | 3:QC:140:ARG:HB2   | 2.25                     | 0.65              |
| 19:QS:3:ARG:CZ     | 19:QS:8:GLY:HA2    | 2.26                     | 0.65              |
| 25:RA:443:A:N7     | 29:RF:45:ARG:HD2   | 2.11                     | 0.65              |
| 27:RD:237:GLU:N    | 27:RD:237:GLU:OE1  | 2.29                     | 0.65              |
| 32:RI:4:ILE:HD11   | 32:RI:44:LEU:HD12  | 1.78                     | 0.65              |
| 41:RV:76:LYS:HB2   | 41:RV:81:TYR:HB3   | 1.79                     | 0.65              |
| 43:RX:65:ARG:HD3   | 43:RX:65:ARG:N     | 2.12                     | 0.65              |
| 44:RY:60:PHE:O     | 44:RY:61:ILE:HD12  | 1.96                     | 0.65              |
| 2:XB:14:GLY:O      | 2:XB:15:VAL:HG13   | 1.96                     | 0.65              |
| 2:XB:132:LYS:HA    | 2:XB:135:GLN:CD    | 2.22                     | 0.65              |
| 25:YA:33:U:O4      | 25:YA:446:G:O2'    | 2.13                     | 0.65              |
| 28:YE:13:ARG:NH1   | 28:YE:21:VAL:HG12  | 2.11                     | 0.65              |
| 28:YE:101:ARG:CZ   | 28:YE:171:GLU:HB2  | 2.25                     | 0.65              |
| 31:YH:168:PRO:O    | 31:YH:169:VAL:HG12 | 1.96                     | 0.65              |
| 35:YP:90:ARG:NE    | 35:YP:91:PHE:HD1   | 1.93                     | 0.65              |
| 44:YY:42:VAL:CG1   | 44:YY:65:ALA:HB3   | 2.26                     | 0.65              |
| 1:QA:1298:C:OP2    | 7:QG:114:ARG:NH2   | 2.29                     | 0.65              |
| 10:QJ:38:ILE:HD11  | 10:QJ:71:LEU:HB3   | 1.78                     | 0.65              |
| 12:QL:115:LYS:O    | 12:QL:117:ARG:HG3  | 1.96                     | 0.65              |
| 25:RA:2832:U:H4'   | 25:RA:2833:G:H5''  | 1.78                     | 0.65              |
| 27:RD:27:THR:CG2   | 27:RD:28:GLU:H     | 2.09                     | 0.65              |
| 31:RH:128:PRO:CD   | 31:RH:129:THR:H    | 2.09                     | 0.65              |
| 34:RO:113:LYS:O    | 34:RO:117:LEU:HD12 | 1.96                     | 0.65              |
| 35:RP:138:LEU:HD11 | 35:RP:144:GLU:HG3  | 1.78                     | 0.65              |
| 1:XA:677:U:H3      | 1:XA:713:G:H22     | 1.44                     | 0.65              |
| 7:XG:140:ASP:C     | 7:XG:142:GLU:H     | 2.03                     | 0.65              |
| 15:XO:8:LYS:O      | 15:XO:12:ILE:HG13  | 1.96                     | 0.65              |
| 20:XT:36:LEU:HD12  | 20:XT:55:ILE:HG23  | 1.76                     | 0.65              |
| 27:YD:27:THR:CG2   | 27:YD:28:GLU:H     | 2.08                     | 0.65              |
| 34:YO:71:ARG:NH1   | 39:YT:74:ARG:HH21  | 1.94                     | 0.65              |
| 35:YP:39:LYS:HA    | 35:YP:45:LEU:HD13  | 1.79                     | 0.65              |
| 37:YR:26:LYS:HE2   | 37:YR:70:LEU:O     | 1.95                     | 0.65              |
| 1:QA:963:G:H21     | 10:QJ:55:LYS:HD3   | 1.61                     | 0.65              |
| 1:QA:1314:C:OP1    | 19:QS:6:LYS:HE3    | 1.96                     | 0.65              |
| 2:QB:164:VAL:HB    | 2:QB:186:ALA:HB2   | 1.78                     | 0.65              |
| 4:QD:28:SER:CB     | 4:QD:29:PRO:HD3    | 2.25                     | 0.65              |
| 4:QD:52:SER:O      | 4:QD:56:VAL:HG23   | 1.95                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:122:ARG:O     | 4:QD:122:ARG:HD3   | 1.97                     | 0.65              |
| 9:QI:28:VAL:HA     | 9:QI:63:ILE:HB     | 1.79                     | 0.65              |
| 16:QP:45:THR:HG22  | 16:QP:47:ASP:H     | 1.60                     | 0.65              |
| 25:RA:2073:C:HO2'  | 25:RA:2598:A:HO2'  | 1.34                     | 0.65              |
| 25:RA:2818:G:OP2   | 37:RR:42:LYS:NZ    | 2.28                     | 0.65              |
| 28:RE:4:ILE:C      | 28:RE:5:LEU:HD23   | 2.22                     | 0.65              |
| 28:RE:11:MET:HE3   | 28:RE:186:GLY:HA2  | 1.79                     | 0.65              |
| 36:RQ:86:GLY:C     | 36:RQ:88:GLY:N     | 2.52                     | 0.65              |
| 42:RW:25:ARG:NH1   | 42:RW:25:ARG:HB2   | 2.11                     | 0.65              |
| 1:XA:15:G:H4'      | 5:XE:24:ARG:NH1    | 2.12                     | 0.65              |
| 1:XA:939:G:H5''    | 7:XG:102:ARG:NH2   | 2.11                     | 0.65              |
| 2:XB:87:ARG:O      | 2:XB:87:ARG:HD2    | 1.95                     | 0.65              |
| 2:XB:87:ARG:HH11   | 2:XB:223:ILE:CD1   | 2.09                     | 0.65              |
| 10:XJ:99:LYS:O     | 10:XJ:100:THR:HG23 | 1.96                     | 0.65              |
| 12:XL:48:PRO:CD    | 12:XL:49:ASN:H     | 2.10                     | 0.65              |
| 14:XN:23:ARG:NH1   | 14:XN:30:ALA:HB2   | 2.11                     | 0.65              |
| 16:XP:45:THR:HG22  | 16:XP:47:ASP:H     | 1.60                     | 0.65              |
| 17:XQ:74:LEU:HD12  | 17:XQ:75:ARG:HG2   | 1.76                     | 0.65              |
| 19:XS:10:PHE:CG    | 19:XS:11:VAL:N     | 2.64                     | 0.65              |
| 25:YA:2233:U:H2'   | 25:YA:2234:G:C8    | 2.32                     | 0.65              |
| 27:YD:80:ALA:HB3   | 27:YD:94:LEU:CD1   | 2.26                     | 0.65              |
| 4:QD:94:LEU:H      | 4:QD:94:LEU:CD1    | 2.08                     | 0.65              |
| 19:QS:15:LEU:O     | 19:QS:19:VAL:N     | 2.26                     | 0.65              |
| 21:QU:25:LYS:HE2   | 21:QU:26:LYS:O     | 1.96                     | 0.65              |
| 25:RA:2131:G:N2    | 25:RA:2158:A:N7    | 2.44                     | 0.65              |
| 28:RE:28:ALA:O     | 28:RE:93:VAL:HG23  | 1.95                     | 0.65              |
| 32:RI:104:GLN:O    | 32:RI:105:HIS:ND1  | 2.29                     | 0.65              |
| 42:RW:18:ARG:HG3   | 42:RW:76:VAL:HG13  | 1.77                     | 0.65              |
| 1:XA:243:A:H4'     | 1:XA:244:U:H3'     | 1.79                     | 0.65              |
| 6:XF:96:PRO:HB3    | 18:XR:30:ASP:OD2   | 1.95                     | 0.65              |
| 8:XH:118:VAL:C     | 8:XH:119:LEU:HD23  | 2.22                     | 0.65              |
| 9:XI:53:VAL:HG21   | 9:XI:92:TYR:CE1    | 2.32                     | 0.65              |
| 12:XL:39:VAL:HB    | 12:XL:57:LYS:HB2   | 1.78                     | 0.65              |
| 25:YA:910:A:N3     | 25:YA:2264:C:O2'   | 2.28                     | 0.65              |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:O    | 1.96                     | 0.65              |
| 48:Y2:42:GLY:O     | 48:Y2:44:LEU:N     | 2.30                     | 0.65              |
| 1:QA:1104:G:H4'    | 2:QB:111:ARG:NH1   | 2.11                     | 0.65              |
| 2:QB:17:PHE:HD2    | 2:QB:44:LEU:HD21   | 1.61                     | 0.65              |
| 2:QB:132:LYS:HA    | 2:QB:135:GLN:CD    | 2.22                     | 0.65              |
| 4:QD:13:ARG:HD3    | 4:QD:38:TYR:O      | 1.97                     | 0.65              |
| 5:QE:41:VAL:CG1    | 5:QE:113:ALA:HB2   | 2.25                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:QG:11:GLN:O      | 7:QG:12:LEU:HD13  | 1.97                     | 0.65              |
| 8:QH:20:TYR:HA     | 8:QH:65:TYR:HE2   | 1.60                     | 0.65              |
| 10:QJ:6:ILE:HD11   | 10:QJ:72:VAL:CB   | 2.24                     | 0.65              |
| 10:QJ:34:VAL:HG22  | 10:QJ:74:ILE:HG22 | 1.77                     | 0.65              |
| 12:QL:21:LYS:HD2   | 12:QL:21:LYS:N    | 2.11                     | 0.65              |
| 12:QL:39:VAL:HB    | 12:QL:57:LYS:HB2  | 1.78                     | 0.65              |
| 13:QM:74:VAL:O     | 13:QM:78:ILE:HG13 | 1.96                     | 0.65              |
| 16:QP:6:LEU:HD23   | 16:QP:17:TYR:CD2  | 2.32                     | 0.65              |
| 18:QR:43:PHE:CE2   | 18:QR:58:LEU:HD11 | 2.31                     | 0.65              |
| 19:QS:21:GLU:O     | 19:QS:25:LYS:HB3  | 1.97                     | 0.65              |
| 26:RB:56:G:H5'     | 30:RG:27:ASN:ND2  | 2.12                     | 0.65              |
| 27:RD:176:ARG:HH11 | 27:RD:176:ARG:HG2 | 1.61                     | 0.65              |
| 35:RP:39:LYS:HA    | 35:RP:45:LEU:HD13 | 1.79                     | 0.65              |
| 36:RQ:80:GLU:C     | 36:RQ:81:VAL:HG13 | 2.22                     | 0.65              |
| 36:RQ:88:GLY:C     | 36:RQ:90:VAL:H    | 2.02                     | 0.65              |
| 40:RU:90:VAL:CG1   | 40:RU:91:ASP:H    | 2.00                     | 0.65              |
| 40:RU:96:ALA:C     | 40:RU:98:LEU:H    | 2.03                     | 0.65              |
| 44:RY:35:TYR:CE1   | 44:RY:69:ALA:HB3  | 2.31                     | 0.65              |
| 47:R1:29:GLY:O     | 47:R1:30:VAL:HG23 | 1.97                     | 0.65              |
| 50:R4:49:PHE:O     | 50:R4:50:VAL:HG23 | 1.97                     | 0.65              |
| 2:XB:17:PHE:HD2    | 2:XB:44:LEU:HD21  | 1.61                     | 0.65              |
| 3:XC:70:VAL:HG12   | 3:XC:71:ALA:N     | 2.10                     | 0.65              |
| 6:XF:1:MET:HE1     | 6:XF:68:PRO:HB3   | 1.78                     | 0.65              |
| 6:XF:41:GLU:O      | 6:XF:43:LEU:HD12  | 1.96                     | 0.65              |
| 6:XF:98:LEU:HB3    | 18:XR:30:ASP:HA   | 1.78                     | 0.65              |
| 9:XI:128:ARG:NH2   | 22:XV:35:A:P      | 2.70                     | 0.65              |
| 10:XJ:38:ILE:HD11  | 10:XJ:71:LEU:HB3  | 1.78                     | 0.65              |
| 13:XM:51:ALA:O     | 13:XM:55:ARG:HG3  | 1.97                     | 0.65              |
| 16:XP:21:VAL:HG23  | 16:XP:33:ILE:HB   | 1.77                     | 0.65              |
| 20:XT:83:ARG:CA    | 20:XT:86:ARG:HB3  | 2.27                     | 0.65              |
| 25:YA:1484:G:H1    | 25:YA:1505:C:H42  | 1.45                     | 0.65              |
| 25:YA:1903:G:OP2   | 27:YD:241:PRO:HB2 | 1.97                     | 0.65              |
| 27:YD:176:ARG:HH11 | 27:YD:176:ARG:HG2 | 1.60                     | 0.65              |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:N   | 2.07                     | 0.65              |
| 34:YO:86:ILE:H     | 34:YO:86:ILE:HD12 | 1.61                     | 0.65              |
| 2:QB:155:LEU:HD12  | 2:QB:157:ARG:O    | 1.97                     | 0.65              |
| 5:QE:83:GLU:HG2    | 5:QE:88:LYS:HG3   | 1.78                     | 0.65              |
| 8:QH:118:VAL:C     | 8:QH:119:LEU:HD23 | 2.22                     | 0.65              |
| 10:QJ:27:ALA:CB    | 10:QJ:34:VAL:HG21 | 2.26                     | 0.65              |
| 20:QT:83:ARG:CA    | 20:QT:86:ARG:HB3  | 2.27                     | 0.65              |
| 28:RE:37:ARG:HA    | 28:RE:37:ARG:NE   | 2.11                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:RE:51:PHE:O     | 28:RE:52:LEU:C    | 2.38                     | 0.65              |
| 34:RO:7:TYR:CE1    | 34:RO:20:MET:HB2  | 2.32                     | 0.65              |
| 34:RO:12:ASP:OD1   | 34:RO:14:THR:HG23 | 1.97                     | 0.65              |
| 47:R1:11:ARG:HB3   | 47:R1:11:ARG:HH11 | 1.61                     | 0.65              |
| 2:XB:67:THR:HG21   | 2:XB:155:LEU:CD2  | 2.27                     | 0.65              |
| 3:XC:101:LEU:HD23  | 3:XC:102:ASN:N    | 2.11                     | 0.65              |
| 4:XD:52:SER:HB3    | 4:XD:55:ALA:CB    | 2.27                     | 0.65              |
| 7:XG:21:VAL:HG23   | 7:XG:22:LEU:H     | 1.61                     | 0.65              |
| 12:XL:115:LYS:O    | 12:XL:117:ARG:HG3 | 1.96                     | 0.65              |
| 14:YN:40:CYS:SG    | 14:YN:43:CYS:CB   | 2.83                     | 0.65              |
| 15:XO:74:ASP:OD1   | 15:XO:77:ARG:N    | 2.30                     | 0.65              |
| 19:XS:9:VAL:HG12   | 50:Y4:66:SER:O    | 1.96                     | 0.65              |
| 19:XS:21:GLU:HG3   | 19:XS:22:LEU:N    | 2.11                     | 0.65              |
| 1:QA:1446:A:O2'    | 1:QA:1447:G:O5'   | 2.14                     | 0.65              |
| 3:QC:70:VAL:HG12   | 3:QC:71:ALA:N     | 2.10                     | 0.65              |
| 6:QF:50:TYR:CE1    | 18:QR:77:GLY:HA2  | 2.32                     | 0.65              |
| 15:QO:74:ASP:OD1   | 15:QO:77:ARG:N    | 2.30                     | 0.65              |
| 16:QP:51:VAL:HG21  | 16:QP:77:ALA:HB2  | 1.78                     | 0.65              |
| 20:QT:44:ALA:HB2   | 20:QT:88:VAL:HG13 | 1.78                     | 0.65              |
| 25:RA:77:C:O3'     | 48:R2:14:ARG:NH2  | 2.30                     | 0.65              |
| 29:RF:155:LEU:HD13 | 29:RF:174:VAL:CG1 | 2.27                     | 0.65              |
| 34:RO:71:ARG:NH1   | 39:RT:74:ARG:HH21 | 1.94                     | 0.65              |
| 47:R1:56:GLN:N     | 47:R1:56:GLN:HE21 | 1.93                     | 0.65              |
| 50:R4:36:CYS:O     | 50:R4:37:SER:O    | 2.14                     | 0.65              |
| 51:R5:56:LYS:H     | 51:R5:56:LYS:CD   | 2.07                     | 0.65              |
| 1:XA:565:U:H5''    | 1:XA:566:G:H2'    | 1.78                     | 0.65              |
| 19:XS:3:ARG:CZ     | 19:XS:8:GLY:HA2   | 2.26                     | 0.65              |
| 25:YA:247:G:O6     | 54:Y8:12:LYS:NZ   | 2.22                     | 0.65              |
| 35:YP:97:PRO:HD3   | 35:YP:126:VAL:O   | 1.97                     | 0.65              |
| 39:YT:11:GLU:N     | 39:YT:11:GLU:OE1  | 2.27                     | 0.65              |
| 44:YY:99:CYS:SG    | 44:YY:100:ALA:N   | 2.69                     | 0.65              |
| 47:Y1:80:LEU:C     | 47:Y1:81:LYS:CD   | 2.69                     | 0.65              |
| 54:Y8:52:LYS:O     | 54:Y8:52:LYS:HG3  | 1.97                     | 0.65              |
| 4:QD:52:SER:HB3    | 4:QD:55:ALA:CB    | 2.27                     | 0.65              |
| 6:QF:98:LEU:HB3    | 18:QR:30:ASP:HA   | 1.79                     | 0.65              |
| 15:QO:8:LYS:O      | 15:QO:12:ILE:HG13 | 1.97                     | 0.65              |
| 27:RD:172:TYR:HB3  | 27:RD:184:LYS:HG2 | 1.77                     | 0.65              |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:NZ   | 2.11                     | 0.65              |
| 35:RP:6:LEU:O      | 35:RP:7:ARG:HG2   | 1.97                     | 0.65              |
| 35:RP:138:LEU:C    | 35:RP:140:ALA:N   | 2.55                     | 0.65              |
| 40:RU:74:LEU:HD23  | 40:RU:114:LYS:HD3 | 1.78                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:R1:80:LEU:C    | 47:R1:81:LYS:CD    | 2.69                     | 0.65              |
| 48:R2:40:SER:C    | 48:R2:42:GLY:N     | 2.51                     | 0.65              |
| 48:R2:69:ARG:HB2  | 48:R2:69:ARG:NH1   | 2.11                     | 0.65              |
| 1:XA:501:C:OP1    | 12:XL:117:ARG:NH2  | 2.29                     | 0.65              |
| 1:XA:1008:C:H42   | 1:XA:1021:G:H1     | 1.44                     | 0.65              |
| 7:XG:11:GLN:O     | 7:XG:12:LEU:HD13   | 1.97                     | 0.65              |
| 13:XM:23:TYR:CB   | 13:XM:67:GLU:HG2   | 2.25                     | 0.65              |
| 15:XO:25:THR:HG21 | 15:XO:70:LEU:HB2   | 1.77                     | 0.65              |
| 16:XP:6:LEU:HD23  | 16:XP:17:TYR:CD2   | 2.32                     | 0.65              |
| 25:YA:2723:C:O3'  | 37:YR:1:MET:HE3    | 1.96                     | 0.65              |
| 33:YN:43:THR:HB   | 33:YN:46:VAL:CG1   | 2.27                     | 0.65              |
| 35:YP:6:LEU:O     | 35:YP:7:ARG:HG2    | 1.97                     | 0.65              |
| 35:YP:113:LYS:HG2 | 35:YP:115:LEU:HD23 | 1.79                     | 0.65              |
| 48:Y2:69:ARG:NH1  | 48:Y2:69:ARG:HB2   | 2.11                     | 0.65              |
| 1:QA:184:G:H2'    | 1:QA:185:A:H8      | 1.61                     | 0.65              |
| 8:QH:20:TYR:CE2   | 8:QH:75:ARG:HD2    | 2.32                     | 0.65              |
| 10:QJ:39:PRO:HB3  | 10:QJ:70:ARG:HH12  | 1.61                     | 0.65              |
| 17:QQ:41:LYS:HZ3  | 17:QQ:92:ARG:HH22  | 1.45                     | 0.65              |
| 25:RA:2419:U:H5'  | 52:R6:23:THR:HG22  | 1.78                     | 0.65              |
| 28:RE:13:ARG:NH1  | 28:RE:21:VAL:HG12  | 2.11                     | 0.65              |
| 52:R6:27:LYS:HB2  | 52:R6:27:LYS:HZ3   | 1.60                     | 0.65              |
| 2:XB:7:VAL:HG22   | 2:XB:8:LYS:HD3     | 1.77                     | 0.65              |
| 5:XE:50:GLU:HG3   | 5:XE:52:PRO:HD2    | 1.79                     | 0.65              |
| 6:XF:97:PHE:HD2   | 6:XF:97:PHE:C      | 2.05                     | 0.65              |
| 7:XG:141:VAL:HG12 | 7:XG:141:VAL:O     | 1.95                     | 0.65              |
| 12:XL:21:LYS:N    | 12:XL:21:LYS:HD2   | 2.11                     | 0.65              |
| 25:YA:2287:A:H62  | 25:YA:2344:U:H3    | 1.43                     | 0.65              |
| 27:YD:44:ASN:HB3  | 27:YD:49:ILE:HG22  | 1.78                     | 0.65              |
| 27:YD:77:ALA:HB2  | 27:YD:97:TYR:HA    | 1.77                     | 0.65              |
| 28:YE:10:GLY:H    | 28:YE:25:VAL:HG23  | 1.60                     | 0.65              |
| 31:YH:128:PRO:CD  | 31:YH:129:THR:H    | 2.09                     | 0.65              |
| 36:YQ:23:GLY:HA3  | 36:YQ:101:ARG:NH1  | 2.12                     | 0.65              |
| 37:YR:28:LEU:HD21 | 37:YR:114:VAL:HG12 | 1.79                     | 0.65              |
| 39:YT:22:PHE:N    | 39:YT:22:PHE:CD2   | 2.64                     | 0.65              |
| 40:YU:74:LEU:HD23 | 40:YU:114:LYS:HD3  | 1.78                     | 0.65              |
| 42:YW:59:VAL:HG12 | 42:YW:60:ASN:N     | 2.11                     | 0.65              |
| 54:Y8:56:GLU:N    | 54:Y8:56:GLU:OE1   | 2.30                     | 0.65              |
| 1:QA:1321:C:H3'   | 1:QA:1322:C:H5''   | 1.79                     | 0.64              |
| 2:QB:14:GLY:O     | 2:QB:15:VAL:HG13   | 1.96                     | 0.64              |
| 7:QG:21:VAL:HG23  | 7:QG:22:LEU:H      | 1.60                     | 0.64              |
| 12:QL:26:ALA:O    | 12:QL:27:LEU:O     | 2.14                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:QS:10:PHE:CG    | 19:QS:11:VAL:N    | 2.65                     | 0.64              |
| 19:QS:69:HIS:ND1   | 50:R4:69:LYS:HE2  | 2.12                     | 0.64              |
| 25:RA:323:G:H2'    | 29:RF:169:ASN:OD1 | 1.97                     | 0.64              |
| 29:RF:45:ARG:CG    | 29:RF:45:ARG:HH11 | 2.10                     | 0.64              |
| 31:RH:51:ARG:HH11  | 31:RH:51:ARG:HG3  | 1.61                     | 0.64              |
| 35:RP:97:PRO:HD3   | 35:RP:126:VAL:O   | 1.97                     | 0.64              |
| 41:RV:43:GLU:OE2   | 41:RV:43:GLU:HA   | 1.95                     | 0.64              |
| 47:R1:73:LEU:C     | 47:R1:75:GLU:H    | 2.03                     | 0.64              |
| 1:XA:128:G:O2'     | 17:XQ:3:LYS:NZ    | 2.29                     | 0.64              |
| 2:XB:164:VAL:HB    | 2:XB:186:ALA:HB2  | 1.78                     | 0.64              |
| 3:XC:34:LEU:HD21   | 3:XC:38:ARG:HD2   | 1.79                     | 0.64              |
| 4:XD:122:ARG:HD3   | 4:XD:122:ARG:O    | 1.97                     | 0.64              |
| 5:XE:41:VAL:HG12   | 5:XE:112:LEU:O    | 1.97                     | 0.64              |
| 9:XI:112:LYS:HA    | 9:XI:119:ALA:HB2  | 1.77                     | 0.64              |
| 13:XM:65:LYS:NZ    | 50:Y4:52:THR:HG21 | 2.11                     | 0.64              |
| 25:YA:1006:C:H1'   | 33:YN:106:MET:CE  | 2.27                     | 0.64              |
| 25:YA:2396:G:OP1   | 47:Y1:25:LYS:NZ   | 2.30                     | 0.64              |
| 35:YP:138:LEU:HD11 | 35:YP:144:GLU:HG3 | 1.79                     | 0.64              |
| 42:YW:25:ARG:HB2   | 42:YW:25:ARG:NH1  | 2.11                     | 0.64              |
| 50:Y4:36:CYS:O     | 50:Y4:37:SER:O    | 2.14                     | 0.64              |
| 1:QA:156:G:H1      | 1:QA:165:C:H42    | 1.46                     | 0.64              |
| 6:QF:97:PHE:C      | 6:QF:97:PHE:HD2   | 2.05                     | 0.64              |
| 25:RA:2372:G:H4'   | 52:R6:46:HIS:CD2  | 2.32                     | 0.64              |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:CG2 | 2.27                     | 0.64              |
| 34:RO:110:GLY:HA2  | 34:RO:112:MET:HE3 | 1.77                     | 0.64              |
| 37:RR:75:LEU:HD13  | 37:RR:75:LEU:C    | 2.22                     | 0.64              |
| 51:R5:40:LYS:HD3   | 51:R5:46:CYS:CB   | 2.26                     | 0.64              |
| 1:XA:523:A:H61     | 12:XL:92:ASP:HB2  | 1.62                     | 0.64              |
| 5:XE:41:VAL:CG1    | 5:XE:113:ALA:HB2  | 2.25                     | 0.64              |
| 8:XH:20:TYR:CE2    | 8:XH:75:ARG:HD2   | 2.32                     | 0.64              |
| 14:XN:19:ARG:O     | 14:XN:20:ALA:C    | 2.40                     | 0.64              |
| 18:XR:73:ALA:HB3   | 18:XR:79:LEU:HD12 | 1.78                     | 0.64              |
| 19:XS:21:GLU:O     | 19:XS:25:LYS:HB3  | 1.97                     | 0.64              |
| 19:XS:65:ASN:N     | 19:XS:65:ASN:HD22 | 1.94                     | 0.64              |
| 25:YA:2415:G:H4'   | 35:YP:67:MET:N    | 2.13                     | 0.64              |
| 30:YG:81:LYS:O     | 30:YG:82:LEU:HB2  | 1.95                     | 0.64              |
| 31:YH:105:LEU:H    | 31:YH:105:LEU:CD1 | 2.09                     | 0.64              |
| 36:YQ:81:VAL:O     | 36:YQ:82:ARG:HG2  | 1.97                     | 0.64              |
| 40:YU:102:GLU:HG3  | 41:YV:2:PHE:HE2   | 1.62                     | 0.64              |
| 41:YV:43:GLU:HA    | 41:YV:43:GLU:OE2  | 1.95                     | 0.64              |
| 51:Y5:40:LYS:HD3   | 51:Y5:46:CYS:CB   | 2.26                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:163:GLU:C     | 4:QD:165:MET:H     | 2.03                     | 0.64              |
| 19:QS:35:SER:O     | 19:QS:71:LEU:HD12  | 1.96                     | 0.64              |
| 25:RA:2392:A:C8    | 35:RP:60:MET:HG3   | 2.32                     | 0.64              |
| 25:RA:2438:U:O3'   | 25:RA:2439:A:H3'   | 1.98                     | 0.64              |
| 25:RA:2637:U:H5''  | 28:RE:82:ARG:HH21  | 1.62                     | 0.64              |
| 28:RE:35:GLN:CG    | 28:RE:37:ARG:HE    | 2.11                     | 0.64              |
| 28:RE:50:GLY:HA3   | 28:RE:74:PRO:HG3   | 1.79                     | 0.64              |
| 31:RH:105:LEU:H    | 31:RH:105:LEU:CD1  | 2.09                     | 0.64              |
| 31:RH:148:ILE:O    | 31:RH:151:ILE:HG12 | 1.98                     | 0.64              |
| 36:RQ:81:VAL:O     | 36:RQ:82:ARG:HG2   | 1.97                     | 0.64              |
| 39:RT:11:GLU:N     | 39:RT:11:GLU:OE1   | 2.27                     | 0.64              |
| 40:RU:65:ILE:HG12  | 40:RU:96:ALA:CB    | 2.26                     | 0.64              |
| 1:XA:67:C:H2'      | 1:XA:68:G:C8       | 2.32                     | 0.64              |
| 1:XA:1347:G:C8     | 9:XI:107:ARG:HB3   | 2.32                     | 0.64              |
| 11:XK:103:LEU:HD22 | 11:XK:103:LEU:H    | 1.62                     | 0.64              |
| 14:YN:7:ILE:HG13   | 14:YN:8:GLU:N      | 2.11                     | 0.64              |
| 20:XT:44:ALA:HB2   | 20:XT:88:VAL:HG13  | 1.78                     | 0.64              |
| 25:YA:1007:C:O3'   | 33:YN:108:PRO:HB3  | 1.97                     | 0.64              |
| 29:YF:155:LEU:HD13 | 29:YF:174:VAL:CG1  | 2.27                     | 0.64              |
| 30:YG:114:ILE:CG2  | 30:YG:117:PHE:HB2  | 2.27                     | 0.64              |
| 35:YP:98:GLU:O     | 35:YP:101:VAL:HG12 | 1.98                     | 0.64              |
| 2:QB:67:THR:HG21   | 2:QB:155:LEU:CD2   | 2.27                     | 0.64              |
| 3:QC:58:GLU:O      | 3:QC:64:VAL:HA     | 1.98                     | 0.64              |
| 16:QP:58:TYR:O     | 16:QP:62:VAL:HG22  | 1.96                     | 0.64              |
| 25:RA:1059:G:O6    | 25:RA:1079:C:N4    | 2.30                     | 0.64              |
| 27:RD:236:GLY:C    | 27:RD:237:GLU:OE1  | 2.39                     | 0.64              |
| 30:RG:81:LYS:O     | 30:RG:82:LEU:HB2   | 1.96                     | 0.64              |
| 33:RN:57:ALA:HA    | 33:RN:60:ILE:HD11  | 1.77                     | 0.64              |
| 47:R1:80:LEU:HD12  | 47:R1:81:LYS:HE3   | 1.78                     | 0.64              |
| 1:XA:1200:C:H4'    | 1:XA:1201:A:H5'    | 1.80                     | 0.64              |
| 4:XD:61:LYS:HD2    | 4:XD:206:PHE:CE2   | 2.32                     | 0.64              |
| 5:XE:83:GLU:HG2    | 5:XE:88:LYS:HG3    | 1.78                     | 0.64              |
| 21:XU:25:LYS:HE2   | 21:XU:26:LYS:O     | 1.96                     | 0.64              |
| 25:YA:1287:A:N7    | 37:YR:107:ASP:HB2  | 2.13                     | 0.64              |
| 29:YF:175:THR:O    | 29:YF:176:LEU:HB2  | 1.96                     | 0.64              |
| 30:YG:82:LEU:HA    | 30:YG:86:MET:SD    | 2.38                     | 0.64              |
| 31:YH:117:PRO:HB3  | 31:YH:123:PHE:CE1  | 2.33                     | 0.64              |
| 34:YO:12:ASP:OD1   | 34:YO:14:THR:HG23  | 1.97                     | 0.64              |
| 45:YZ:144:LEU:HD11 | 45:YZ:149:SER:HA   | 1.78                     | 0.64              |
| 2:QB:158:LEU:O     | 2:QB:158:LEU:HD12  | 1.98                     | 0.64              |
| 3:QC:138:VAL:HG13  | 3:QC:149:ALA:CB    | 2.27                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:QD:61:LYS:HD2   | 4:QD:206:PHE:CE2   | 2.32                     | 0.64              |
| 9:QI:53:VAL:HG21  | 9:QI:92:TYR:CE1    | 2.32                     | 0.64              |
| 10:QJ:80:LYS:HE2  | 1:XA:1162:C:O2'    | 1.97                     | 0.64              |
| 14:QN:7:ILE:HG13  | 14:QN:8:GLU:N      | 2.11                     | 0.64              |
| 16:QP:21:VAL:HG23 | 16:QP:33:ILE:HB    | 1.78                     | 0.64              |
| 24:QX:6:G:O2'     | 24:QX:7:G:OP1      | 2.10                     | 0.64              |
| 26:RB:38:C:H42    | 26:RB:44:G:H1      | 1.46                     | 0.64              |
| 27:RD:35:LYS:HE3  | 27:RD:64:ILE:C     | 2.21                     | 0.64              |
| 27:RD:77:ALA:HB2  | 27:RD:97:TYR:HA    | 1.77                     | 0.64              |
| 33:RN:15:LEU:HD12 | 33:RN:136:GLU:HB2  | 1.79                     | 0.64              |
| 42:RW:86:LEU:HD12 | 42:RW:87:PRO:CD    | 2.23                     | 0.64              |
| 50:R4:71:ARG:HH11 | 50:R4:71:ARG:CG    | 1.98                     | 0.64              |
| 54:R8:56:GLU:N    | 54:R8:56:GLU:OE1   | 2.30                     | 0.64              |
| 10:XJ:27:ALA:CB   | 10:XJ:34:VAL:HG21  | 2.26                     | 0.64              |
| 25:YA:2393:A:H4'  | 35:YP:61:ARG:O     | 1.96                     | 0.64              |
| 28:YE:69:LYS:O    | 28:YE:71:GLY:N     | 2.27                     | 0.64              |
| 36:YQ:86:GLY:C    | 36:YQ:88:GLY:N     | 2.52                     | 0.64              |
| 37:YR:75:LEU:HD13 | 37:YR:75:LEU:C     | 2.22                     | 0.64              |
| 41:YV:76:LYS:HB2  | 41:YV:81:TYR:HB3   | 1.79                     | 0.64              |
| 44:YY:86:ARG:O    | 44:YY:92:ASN:HB2   | 1.97                     | 0.64              |
| 47:Y1:29:GLY:O    | 47:Y1:30:VAL:HG23  | 1.97                     | 0.64              |
| 50:Y4:35:VAL:O    | 50:Y4:37:SER:N     | 2.26                     | 0.64              |
| 1:QA:474:G:H5'    | 16:QP:81:ARG:HG3   | 1.78                     | 0.64              |
| 1:QA:1152:A:OP1   | 10:QJ:68:HIS:NE2   | 2.30                     | 0.64              |
| 3:QC:34:LEU:HD21  | 3:QC:38:ARG:HD2    | 1.79                     | 0.64              |
| 4:QD:29:PRO:HG2   | 4:QD:30:LYS:NZ     | 2.12                     | 0.64              |
| 4:QD:170:VAL:HG22 | 4:QD:171:GLY:N     | 2.12                     | 0.64              |
| 11:QK:103:LEU:H   | 11:QK:103:LEU:HD22 | 1.62                     | 0.64              |
| 22:QV:6:G:H1      | 22:QV:67:C:H42     | 1.45                     | 0.64              |
| 27:RD:182:LEU:H   | 27:RD:272:ALA:HB3  | 1.62                     | 0.64              |
| 30:RG:82:LEU:HA   | 30:RG:86:MET:SD    | 2.38                     | 0.64              |
| 36:RQ:10:ARG:O    | 36:RQ:11:LYS:HB2   | 1.98                     | 0.64              |
| 37:RR:2:ARG:HG2   | 37:RR:5:LYS:NZ     | 2.13                     | 0.64              |
| 40:RU:102:GLU:HG3 | 41:RV:2:PHE:HE2    | 1.62                     | 0.64              |
| 42:RW:59:VAL:HG12 | 42:RW:60:ASN:N     | 2.11                     | 0.64              |
| 44:RY:56:PRO:HG2  | 44:RY:57:GLN:OE1   | 1.98                     | 0.64              |
| 1:XA:130:A:N3     | 1:XA:263:A:O2'     | 2.31                     | 0.64              |
| 4:XD:13:ARG:HD2   | 4:XD:38:TYR:O      | 1.98                     | 0.64              |
| 8:XH:42:GLU:HG3   | 8:XH:109:ILE:HD12  | 1.80                     | 0.64              |
| 13:XM:8:GLU:OE1   | 30:YG:115:ARG:CZ   | 2.45                     | 0.64              |
| 13:XM:13:LYS:HA   | 13:XM:44:ARG:HD2   | 1.77                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:XP:58:TYR:O     | 16:XP:62:VAL:HG22 | 1.96                     | 0.64              |
| 17:XQ:11:VAL:HG23  | 17:XQ:20:THR:HB   | 1.79                     | 0.64              |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:CG2 | 2.27                     | 0.64              |
| 29:YF:45:ARG:CG    | 29:YF:45:ARG:HH11 | 2.09                     | 0.64              |
| 31:YH:51:ARG:HG3   | 31:YH:51:ARG:HH11 | 1.61                     | 0.64              |
| 31:YH:92:ILE:HD12  | 31:YH:92:ILE:H    | 1.63                     | 0.64              |
| 33:YN:1:MET:HE2    | 41:YV:12:TYR:HA   | 1.80                     | 0.64              |
| 41:YV:36:PRO:HA    | 41:YV:56:SER:OG   | 1.98                     | 0.64              |
| 44:YY:56:PRO:HG2   | 44:YY:57:GLN:OE1  | 1.98                     | 0.64              |
| 2:QB:60:ASP:HB3    | 2:QB:64:ARG:NH1   | 2.13                     | 0.64              |
| 2:QB:134:GLU:HA    | 2:QB:137:ARG:HB3  | 1.80                     | 0.64              |
| 6:QF:12:PRO:HG2    | 6:QF:13:ASN:H     | 1.62                     | 0.64              |
| 13:QM:4:ILE:H      | 13:QM:9:ILE:HG22  | 1.62                     | 0.64              |
| 18:QR:73:ALA:HB3   | 18:QR:79:LEU:HD12 | 1.78                     | 0.64              |
| 25:RA:2393:A:H4'   | 35:RP:61:ARG:O    | 1.98                     | 0.64              |
| 43:RX:11:PRO:HB3   | 43:RX:92:LEU:HD21 | 1.78                     | 0.64              |
| 46:R0:50:ASN:ND2   | 46:R0:81:VAL:O    | 2.27                     | 0.64              |
| 51:R5:40:LYS:NZ    | 51:R5:48:GLU:HB2  | 2.10                     | 0.64              |
| 2:XB:187:LEU:HD12  | 2:XB:205:ASP:HA   | 1.80                     | 0.64              |
| 7:XG:113:GLU:CG    | 7:XG:119:ARG:HG2  | 2.28                     | 0.64              |
| 9:XI:5:TYR:O       | 9:XI:84:ALA:HA    | 1.98                     | 0.64              |
| 12:XL:126:LYS:C    | 12:XL:128:ALA:H   | 2.04                     | 0.64              |
| 33:YN:15:LEU:HD12  | 33:YN:136:GLU:HB2 | 1.80                     | 0.64              |
| 34:YO:7:TYR:CE1    | 34:YO:20:MET:HB2  | 2.32                     | 0.64              |
| 36:YQ:80:GLU:C     | 36:YQ:81:VAL:HG13 | 2.22                     | 0.64              |
| 36:YQ:81:VAL:O     | 36:YQ:82:ARG:HD3  | 1.98                     | 0.64              |
| 37:YR:2:ARG:HG2    | 37:YR:5:LYS:NZ    | 2.13                     | 0.64              |
| 38:YS:78:LEU:HD11  | 38:YS:107:GLU:O   | 1.98                     | 0.64              |
| 47:Y1:80:LEU:HD12  | 47:Y1:81:LYS:HE3  | 1.78                     | 0.64              |
| 9:QI:97:LYS:HB3    | 9:QI:98:PRO:HD3   | 1.79                     | 0.64              |
| 36:RQ:30:GLY:HA3   | 36:RQ:106:VAL:O   | 1.98                     | 0.64              |
| 37:RR:79:LEU:HD23  | 37:RR:79:LEU:C    | 2.23                     | 0.64              |
| 40:RU:92:ARG:C     | 40:RU:94:ASN:H    | 2.05                     | 0.64              |
| 3:XC:181:ASN:ND2   | 3:XC:204:LEU:HB2  | 2.13                     | 0.64              |
| 6:XF:12:PRO:HG2    | 6:XF:13:ASN:H     | 1.62                     | 0.64              |
| 9:XI:28:VAL:HA     | 9:XI:63:ILE:HB    | 1.78                     | 0.64              |
| 11:XK:48:ILE:HD11  | 11:XK:64:ALA:CA   | 2.28                     | 0.64              |
| 25:YA:583:G:OP2    | 40:YU:10:ARG:NH1  | 2.30                     | 0.64              |
| 25:YA:2264:C:O2    | 25:YA:2276:G:N2   | 2.26                     | 0.64              |
| 29:YF:11:VAL:HG12  | 29:YF:12:LEU:N    | 2.13                     | 0.64              |
| 29:YF:46:ARG:HG2   | 29:YF:46:ARG:NH1  | 2.00                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:YH:148:ILE:O   | 31:YH:151:ILE:HG12 | 1.98                     | 0.64              |
| 50:Y4:49:PHE:O    | 50:Y4:50:VAL:HG23  | 1.97                     | 0.64              |
| 3:QC:181:ASN:ND2  | 3:QC:204:LEU:HB2   | 2.13                     | 0.64              |
| 5:QE:41:VAL:HG12  | 5:QE:112:LEU:O     | 1.97                     | 0.64              |
| 12:QL:18:VAL:HG23 | 12:QL:19:ARG:H     | 1.63                     | 0.64              |
| 14:QN:19:ARG:O    | 14:QN:20:ALA:C     | 2.40                     | 0.64              |
| 16:QP:51:VAL:CG1  | 16:QP:52:ASP:H     | 2.11                     | 0.64              |
| 25:RA:2864:G:OP1  | 39:RT:119:LYS:HD2  | 1.96                     | 0.64              |
| 27:RD:12:SER:C    | 27:RD:14:ARG:H     | 2.06                     | 0.64              |
| 45:RZ:97:GLU:HB3  | 45:RZ:125:LEU:HD11 | 1.79                     | 0.64              |
| 47:R1:91:LYS:HG3  | 47:R1:92:LYS:H     | 1.63                     | 0.64              |
| 2:XB:8:LYS:H      | 2:XB:8:LYS:CD      | 2.09                     | 0.64              |
| 2:XB:134:GLU:HA   | 2:XB:137:ARG:HB3   | 1.80                     | 0.64              |
| 3:XC:138:VAL:HG13 | 3:XC:149:ALA:CB    | 2.28                     | 0.64              |
| 9:XI:62:TYR:O     | 9:XI:63:ILE:HD12   | 1.98                     | 0.64              |
| 14:YN:18:VAL:HG23 | 14:YN:19:ARG:H     | 1.63                     | 0.64              |
| 31:YH:3:ARG:HA    | 31:YH:3:ARG:NE     | 2.12                     | 0.64              |
| 36:YQ:86:GLY:C    | 36:YQ:88:GLY:H     | 2.03                     | 0.64              |
| 40:YU:92:ARG:C    | 40:YU:94:ASN:H     | 2.05                     | 0.64              |
| 9:QI:47:LEU:N     | 9:QI:47:LEU:HD22   | 2.13                     | 0.64              |
| 19:QS:21:GLU:HG3  | 19:QS:22:LEU:N     | 2.11                     | 0.64              |
| 21:QU:15:ARG:HH11 | 21:QU:15:ARG:HG2   | 1.63                     | 0.64              |
| 30:RG:114:ILE:CG2 | 30:RG:117:PHE:HB2  | 2.28                     | 0.64              |
| 31:RH:92:ILE:H    | 31:RH:92:ILE:HD12  | 1.63                     | 0.64              |
| 33:RN:1:MET:HE1   | 40:RU:95:LEU:CD2   | 2.18                     | 0.64              |
| 35:RP:105:LEU:O   | 35:RP:106:LEU:CB   | 2.42                     | 0.64              |
| 36:RQ:23:GLY:HA3  | 36:RQ:101:ARG:NH1  | 2.12                     | 0.64              |
| 36:RQ:104:PHE:O   | 36:RQ:105:GLU:HB3  | 1.98                     | 0.64              |
| 5:XE:53:LEU:HD12  | 5:XE:53:LEU:N      | 2.09                     | 0.64              |
| 25:YA:2250:G:C6   | 36:YQ:82:ARG:HD2   | 2.33                     | 0.64              |
| 27:YD:12:SER:C    | 27:YD:14:ARG:H     | 2.06                     | 0.64              |
| 27:YD:135:PHE:N   | 27:YD:135:PHE:HD2  | 1.96                     | 0.64              |
| 28:YE:4:ILE:C     | 28:YE:5:LEU:HD23   | 2.22                     | 0.64              |
| 33:YN:41:ASP:O    | 33:YN:48:MET:HE3   | 1.98                     | 0.64              |
| 34:YO:104:ARG:HG2 | 34:YO:104:ARG:NH1  | 2.13                     | 0.64              |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:HD1   | 1.63                     | 0.64              |
| 38:YS:42:ASP:C    | 38:YS:44:LYS:H     | 2.06                     | 0.64              |
| 43:YX:57:LEU:HD12 | 43:YX:78:LYS:HB2   | 1.77                     | 0.64              |
| 47:Y1:82:LEU:CD1  | 47:Y1:83:GLU:CA    | 2.76                     | 0.64              |
| 54:Y8:48:PHE:N    | 54:Y8:48:PHE:CD1   | 2.66                     | 0.64              |
| 4:QD:166:LYS:HD2  | 27:YD:134:ARG:NH1  | 2.01                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:QJ:42:THR:HG23  | 10:QJ:68:HIS:HA    | 1.80                     | 0.63              |
| 13:QM:51:ALA:O     | 13:QM:55:ARG:HG3   | 1.97                     | 0.63              |
| 14:QN:53:LEU:HB3   | 14:QN:56:VAL:HG21  | 1.80                     | 0.63              |
| 20:QT:26:ASN:HB2   | 20:QT:71:THR:HG23  | 1.79                     | 0.63              |
| 28:RE:201:THR:HG21 | 28:RE:203:LYS:HB3  | 1.80                     | 0.63              |
| 34:RO:86:ILE:HD12  | 34:RO:86:ILE:N     | 2.13                     | 0.63              |
| 35:RP:98:GLU:O     | 35:RP:101:VAL:HG12 | 1.98                     | 0.63              |
| 38:RS:42:ASP:C     | 38:RS:44:LYS:H     | 2.06                     | 0.63              |
| 43:RX:63:LYS:O     | 43:RX:64:LYS:HD2   | 1.98                     | 0.63              |
| 1:XA:1128:C:N3     | 1:XA:1144:G:N2     | 2.46                     | 0.63              |
| 2:XB:21:ARG:HB2    | 2:XB:39:ILE:HA     | 1.80                     | 0.63              |
| 6:XF:50:TYR:CE1    | 18:XR:77:GLY:HA2   | 2.32                     | 0.63              |
| 8:XH:28:ALA:HB3    | 8:XH:57:PRO:HB2    | 1.79                     | 0.63              |
| 8:XH:97:VAL:HG13   | 8:XH:98:LYS:N      | 2.13                     | 0.63              |
| 11:XK:12:ARG:HG2   | 11:XK:13:GLN:H     | 1.63                     | 0.63              |
| 11:XK:19:ALA:HA    | 11:XK:32:ILE:HG22  | 1.80                     | 0.63              |
| 16:XP:51:VAL:HG21  | 16:XP:77:ALA:HB2   | 1.79                     | 0.63              |
| 25:YA:2030:A:H4'   | 25:YA:2031:A:H8    | 1.62                     | 0.63              |
| 25:YA:2867:G:O2'   | 25:YA:2868:A:H8    | 1.80                     | 0.63              |
| 27:YD:18:VAL:HG12  | 27:YD:19:ALA:O     | 1.98                     | 0.63              |
| 28:YE:11:MET:HE3   | 28:YE:186:GLY:HA2  | 1.79                     | 0.63              |
| 33:YN:39:ARG:HB3   | 33:YN:41:ASP:OD1   | 1.98                     | 0.63              |
| 40:YU:96:ALA:C     | 40:YU:98:LEU:H     | 2.04                     | 0.63              |
| 14:QN:18:VAL:HG23  | 14:QN:19:ARG:H     | 1.63                     | 0.63              |
| 15:QO:8:LYS:HB2    | 15:QO:8:LYS:NZ     | 2.13                     | 0.63              |
| 25:RA:270(R):G:H1' | 47:R1:78:LYS:HZ1   | 1.62                     | 0.63              |
| 26:RB:32:C:OP2     | 30:RG:96:ARG:NH2   | 2.26                     | 0.63              |
| 27:RD:35:LYS:HZ1   | 27:RD:65:ILE:HA    | 1.62                     | 0.63              |
| 31:RH:117:PRO:HB3  | 31:RH:123:PHE:CE1  | 2.33                     | 0.63              |
| 33:RN:43:THR:HB    | 33:RN:46:VAL:CG1   | 2.27                     | 0.63              |
| 35:RP:113:LYS:HG2  | 35:RP:115:LEU:HD23 | 1.79                     | 0.63              |
| 37:RR:28:LEU:HD21  | 37:RR:114:VAL:HG12 | 1.79                     | 0.63              |
| 42:RW:74:ALA:O     | 42:RW:75:TYR:HB3   | 1.98                     | 0.63              |
| 50:R4:63:TYR:C     | 50:R4:65:ASP:H     | 2.05                     | 0.63              |
| 1:XA:45:U:H2'      | 1:XA:46:G:C8       | 2.34                     | 0.63              |
| 2:XB:158:LEU:O     | 2:XB:158:LEU:HD12  | 1.97                     | 0.63              |
| 3:XC:58:GLU:O      | 3:XC:64:VAL:HA     | 1.98                     | 0.63              |
| 11:XK:91:ARG:HH22  | 18:XR:88:LYS:HZ3   | 1.45                     | 0.63              |
| 19:XS:2:PRO:HB2    | 50:Y4:68:ARG:HH22  | 1.64                     | 0.63              |
| 25:YA:1026:U:H4'   | 25:YA:1027:A:OP1   | 1.99                     | 0.63              |
| 28:YE:14:ILE:CG1   | 28:YE:15:PHE:H     | 2.08                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:YE:201:THR:HG21 | 28:YE:203:LYS:HB3 | 1.80                     | 0.63              |
| 36:YQ:104:PHE:O    | 36:YQ:105:GLU:HB3 | 1.98                     | 0.63              |
| 40:YU:92:ARG:O     | 40:YU:94:ASN:N    | 2.25                     | 0.63              |
| 1:QA:951:G:OP2     | 13:QM:102:ARG:NH2 | 2.31                     | 0.63              |
| 1:QA:1305:G:N2     | 1:QA:1331:G:H2'   | 2.13                     | 0.63              |
| 8:QH:97:VAL:HG13   | 8:QH:98:LYS:N     | 2.13                     | 0.63              |
| 8:QH:112:LEU:HD12  | 8:QH:112:LEU:O    | 1.98                     | 0.63              |
| 20:QT:14:LYS:HA    | 20:QT:17:ARG:NH1  | 2.14                     | 0.63              |
| 25:RA:1803:A:N6    | 25:RA:1814:G:O2'  | 2.30                     | 0.63              |
| 27:RD:135:PHE:N    | 27:RD:135:PHE:HD2 | 1.96                     | 0.63              |
| 31:RH:3:ARG:HA     | 31:RH:3:ARG:NE    | 2.12                     | 0.63              |
| 38:RS:88:ASP:CG    | 38:RS:90:GLY:H    | 2.06                     | 0.63              |
| 41:RV:52:VAL:CG2   | 41:RV:55:ALA:HB3  | 2.28                     | 0.63              |
| 1:XA:522:C:H41     | 12:XL:53:ARG:HH22 | 1.47                     | 0.63              |
| 12:XL:18:VAL:HG23  | 12:XL:19:ARG:H    | 1.62                     | 0.63              |
| 12:XL:62:SER:O     | 12:XL:64:TYR:HD1  | 1.82                     | 0.63              |
| 15:XO:87:ILE:CG2   | 15:XO:88:ARG:H    | 2.00                     | 0.63              |
| 25:YA:807:U:OP2    | 35:YP:41:ARG:NH1  | 2.31                     | 0.63              |
| 35:YP:106:LEU:O    | 35:YP:107:LYS:CB  | 2.46                     | 0.63              |
| 6:QF:62:TRP:C      | 6:QF:63:TYR:HD2   | 2.06                     | 0.63              |
| 11:QK:48:ILE:HD11  | 11:QK:64:ALA:CA   | 2.28                     | 0.63              |
| 19:QS:15:LEU:O     | 19:QS:19:VAL:HG23 | 1.98                     | 0.63              |
| 19:QS:39:THR:HG22  | 19:QS:40:ILE:N    | 2.14                     | 0.63              |
| 29:RF:132:VAL:HG23 | 29:RF:133:ASN:N   | 2.14                     | 0.63              |
| 38:RS:78:LEU:HD11  | 38:RS:107:GLU:O   | 1.98                     | 0.63              |
| 4:XD:165:MET:HE1   | 4:XD:168:ARG:HD2  | 1.80                     | 0.63              |
| 6:XF:97:PHE:C      | 6:XF:97:PHE:CD2   | 2.76                     | 0.63              |
| 9:XI:128:ARG:NH2   | 22:XV:35:A:OP1    | 2.22                     | 0.63              |
| 15:XO:8:LYS:HB2    | 15:XO:8:LYS:NZ    | 2.13                     | 0.63              |
| 20:XT:26:ASN:HB2   | 20:XT:71:THR:HG23 | 1.79                     | 0.63              |
| 24:XX:6:G:O2'      | 24:XX:7:G:OP1     | 2.10                     | 0.63              |
| 27:YD:230:ASP:O    | 27:YD:231:HIS:HB2 | 1.98                     | 0.63              |
| 28:YE:50:GLY:HA3   | 28:YE:74:PRO:HG3  | 1.79                     | 0.63              |
| 29:YF:67:GLN:O     | 29:YF:67:GLN:CG   | 2.32                     | 0.63              |
| 42:YW:110:LYS:HG3  | 42:YW:111:HIS:ND1 | 2.13                     | 0.63              |
| 47:Y1:91:LYS:HG3   | 47:Y1:92:LYS:H    | 1.62                     | 0.63              |
| 50:Y4:63:TYR:C     | 50:Y4:65:ASP:H    | 2.05                     | 0.63              |
| 2:QB:8:LYS:H       | 2:QB:8:LYS:CD     | 2.09                     | 0.63              |
| 2:QB:20:GLU:HB2    | 2:QB:190:THR:OG1  | 1.99                     | 0.63              |
| 5:QE:111:GLU:C     | 5:QE:113:ALA:H    | 2.07                     | 0.63              |
| 8:QH:6:ILE:HB      | 8:QH:85:ARG:HH12  | 1.62                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:QH:28:ALA:HB3    | 8:QH:57:PRO:HB2    | 1.79                     | 0.63              |
| 9:QI:5:TYR:O       | 9:QI:84:ALA:HA     | 1.98                     | 0.63              |
| 27:RD:18:VAL:HG12  | 27:RD:19:ALA:O     | 1.99                     | 0.63              |
| 27:RD:147:LEU:CD1  | 27:RD:155:LEU:HD11 | 2.26                     | 0.63              |
| 33:RN:1:MET:HE2    | 41:RV:12:TYR:HA    | 1.80                     | 0.63              |
| 33:RN:39:ARG:HB3   | 33:RN:41:ASP:OD1   | 1.99                     | 0.63              |
| 33:RN:61:ARG:HA    | 33:RN:61:ARG:HE    | 1.64                     | 0.63              |
| 2:XB:25:ASN:O      | 2:XB:27:LYS:N      | 2.28                     | 0.63              |
| 12:XL:86:ARG:HB2   | 12:XL:101:VAL:CG2  | 2.28                     | 0.63              |
| 18:XR:43:PHE:CE2   | 18:XR:58:LEU:HD11  | 2.31                     | 0.63              |
| 25:YA:1543:A:O2'   | 25:YA:1544:C:O5'   | 2.16                     | 0.63              |
| 35:YP:138:LEU:C    | 35:YP:140:ALA:N    | 2.55                     | 0.63              |
| 39:YT:60:THR:HG22  | 39:YT:77:PRO:HA    | 1.80                     | 0.63              |
| 50:Y4:71:ARG:HH11  | 50:Y4:71:ARG:CG    | 1.98                     | 0.63              |
| 2:QB:37:ASN:C      | 2:QB:39:ILE:H      | 2.07                     | 0.63              |
| 3:QC:95:THR:HG22   | 3:QC:96:GLY:N      | 2.07                     | 0.63              |
| 4:QD:30:LYS:CG     | 4:QD:35:ARG:HE     | 2.11                     | 0.63              |
| 29:RF:28:ILE:HG22  | 29:RF:112:MET:HB3  | 1.80                     | 0.63              |
| 31:RH:153:LYS:HG3  | 31:RH:161:GLY:HA3  | 1.80                     | 0.63              |
| 33:RN:22:THR:CG2   | 33:RN:23:LEU:N     | 2.61                     | 0.63              |
| 35:RP:112:LEU:HD11 | 35:RP:114:ILE:HG23 | 1.81                     | 0.63              |
| 36:RQ:20:ALA:HB1   | 36:RQ:99:PRO:CB    | 2.28                     | 0.63              |
| 36:RQ:66:ILE:CG1   | 36:RQ:67:ARG:H     | 2.12                     | 0.63              |
| 40:RU:102:GLU:HG3  | 41:RV:2:PHE:CE2    | 2.34                     | 0.63              |
| 44:RY:95:LYS:CB    | 44:RY:100:ALA:HA   | 2.13                     | 0.63              |
| 48:R2:42:GLY:O     | 48:R2:44:LEU:N     | 2.30                     | 0.63              |
| 1:XA:1023:G:H3'    | 1:XA:1024:G:H5''   | 1.81                     | 0.63              |
| 2:XB:60:ASP:HB3    | 2:XB:64:ARG:NH1    | 2.13                     | 0.63              |
| 10:XJ:42:THR:HG23  | 10:XJ:68:HIS:HA    | 1.80                     | 0.63              |
| 25:YA:2114:A:N6    | 25:YA:2119:A:N7    | 2.47                     | 0.63              |
| 25:YA:2633:G:H1'   | 28:YE:62:PRO:HG2   | 1.80                     | 0.63              |
| 45:YZ:109:ALA:HB3  | 45:YZ:143:GLY:HA2  | 1.80                     | 0.63              |
| 48:Y2:46:GLN:OE1   | 48:Y2:46:GLN:HA    | 1.97                     | 0.63              |
| 4:QD:30:LYS:HA     | 4:QD:34:GLU:HB2    | 1.79                     | 0.63              |
| 12:QL:62:SER:O     | 12:QL:64:TYR:HD1   | 1.81                     | 0.63              |
| 25:RA:2277:G:H5'   | 36:RQ:85:LYS:HG3   | 1.81                     | 0.63              |
| 25:RA:2466:C:OP1   | 55:R9:4:ARG:HB2    | 1.99                     | 0.63              |
| 28:RE:131:ALA:HB1  | 28:RE:135:HIS:CE1  | 2.34                     | 0.63              |
| 29:RF:11:VAL:HG12  | 29:RF:12:LEU:N     | 2.13                     | 0.63              |
| 36:RQ:81:VAL:O     | 36:RQ:82:ARG:HD3   | 1.98                     | 0.63              |
| 42:RW:110:LYS:HG3  | 42:RW:111:HIS:ND1  | 2.12                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RX:49:VAL:HG13  | 43:RX:83:VAL:HG13  | 1.80                     | 0.63              |
| 47:R1:82:LEU:CD1   | 47:R1:83:GLU:CA    | 2.76                     | 0.63              |
| 2:XB:66:GLY:O      | 2:XB:67:THR:HG23   | 1.99                     | 0.63              |
| 9:XI:118:LYS:O     | 9:XI:119:ALA:HB3   | 1.99                     | 0.63              |
| 16:XP:66:PRO:HG2   | 16:XP:71:ARG:HH12  | 1.64                     | 0.63              |
| 19:XS:15:LEU:O     | 19:XS:19:VAL:HG23  | 1.98                     | 0.63              |
| 27:YD:72:LYS:HG2   | 27:YD:103:ARG:NH2  | 2.13                     | 0.63              |
| 28:YE:35:GLN:CG    | 28:YE:37:ARG:NE    | 2.62                     | 0.63              |
| 35:YP:83:VAL:HG12  | 35:YP:112:LEU:HD21 | 1.81                     | 0.63              |
| 36:YQ:90:VAL:C     | 36:YQ:92:GLY:H     | 2.07                     | 0.63              |
| 37:YR:117:VAL:O    | 37:YR:118:GLU:HB3  | 1.99                     | 0.63              |
| 38:YS:22:GLY:O     | 38:YS:23:ARG:O     | 2.17                     | 0.63              |
| 38:YS:88:ASP:CG    | 38:YS:90:GLY:H     | 2.06                     | 0.63              |
| 39:YT:16:ARG:HE    | 39:YT:19:LEU:HD21  | 1.62                     | 0.63              |
| 1:QA:1175:G:H2'    | 1:QA:1176:A:C8     | 2.33                     | 0.63              |
| 3:QC:3:ASN:N       | 3:QC:3:ASN:HD22    | 1.96                     | 0.63              |
| 3:QC:34:LEU:CD2    | 3:QC:38:ARG:HD2    | 2.29                     | 0.63              |
| 7:QG:9:VAL:CG1     | 7:QG:94:ARG:HE     | 2.12                     | 0.63              |
| 9:QI:59:PHE:HZ     | 9:QI:88:TYR:CE1    | 2.17                     | 0.63              |
| 12:QL:85:ILE:HD11  | 12:QL:98:TYR:HB2   | 1.81                     | 0.63              |
| 12:QL:86:ARG:HB2   | 12:QL:101:VAL:CG2  | 2.28                     | 0.63              |
| 13:QM:40:ASN:HD21  | 13:QM:42:ALA:HB3   | 1.64                     | 0.63              |
| 26:RB:43:C:O5'     | 30:RG:67:LYS:HE3   | 1.98                     | 0.63              |
| 33:RN:41:ASP:O     | 33:RN:48:MET:HE3   | 1.98                     | 0.63              |
| 35:RP:108:LYS:HD2  | 35:RP:108:LYS:H    | 1.64                     | 0.63              |
| 45:RZ:108:PRO:HA   | 45:RZ:142:SER:HA   | 1.80                     | 0.63              |
| 54:R8:48:PHE:N     | 54:R8:48:PHE:CD1   | 2.66                     | 0.63              |
| 2:XB:155:LEU:HD12  | 2:XB:157:ARG:O     | 1.97                     | 0.63              |
| 8:XH:20:TYR:HA     | 8:XH:65:TYR:HE2    | 1.60                     | 0.63              |
| 9:XI:97:LYS:HB3    | 9:XI:98:PRO:HD3    | 1.79                     | 0.63              |
| 11:XK:12:ARG:HG2   | 11:XK:13:GLN:N     | 2.14                     | 0.63              |
| 16:XP:8:ARG:HH11   | 16:XP:8:ARG:HG2    | 1.64                     | 0.63              |
| 30:YG:68:PRO:HB2   | 30:YG:90:LEU:HD12  | 1.80                     | 0.63              |
| 33:YN:7:LYS:H      | 33:YN:7:LYS:HD2    | 1.64                     | 0.63              |
| 33:YN:61:ARG:HA    | 33:YN:61:ARG:HE    | 1.63                     | 0.63              |
| 34:YO:86:ILE:HD12  | 34:YO:86:ILE:N     | 2.13                     | 0.63              |
| 35:YP:13:ASN:C     | 35:YP:15:ARG:N     | 2.54                     | 0.63              |
| 35:YP:114:ILE:HD11 | 35:YP:130:PHE:CD1  | 2.34                     | 0.63              |
| 36:YQ:20:ALA:HB1   | 36:YQ:99:PRO:CB    | 2.29                     | 0.63              |
| 36:YQ:30:GLY:HA3   | 36:YQ:106:VAL:O    | 1.98                     | 0.63              |
| 54:Y8:59:LYS:HZ3   | 54:Y8:59:LYS:HB3   | 1.62                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:1014:A:H4'    | 19:QS:14:HIS:CD2  | 2.33                     | 0.63              |
| 2:QB:187:LEU:HD12  | 2:QB:205:ASP:HA   | 1.79                     | 0.63              |
| 3:QC:70:VAL:HG12   | 3:QC:72:LYS:N     | 2.11                     | 0.63              |
| 3:QC:189:ALA:O     | 3:QC:191:THR:HG23 | 1.99                     | 0.63              |
| 7:QG:113:GLU:CG    | 7:QG:119:ARG:HG2  | 2.28                     | 0.63              |
| 11:QK:19:ALA:HA    | 11:QK:32:ILE:HG22 | 1.80                     | 0.63              |
| 25:RA:660:G:O3'    | 29:RF:38:ARG:NH2  | 2.32                     | 0.63              |
| 25:RA:2747:G:H21   | 25:RA:2757:A:H62  | 1.46                     | 0.63              |
| 27:RD:133:LEU:HD21 | 27:RD:191:ALA:CB  | 2.29                     | 0.63              |
| 37:RR:63:ARG:NH1   | 37:RR:80:PHE:CD1  | 2.67                     | 0.63              |
| 39:RT:16:ARG:HE    | 39:RT:19:LEU:HD21 | 1.63                     | 0.63              |
| 39:RT:60:THR:HG22  | 39:RT:77:PRO:HA   | 1.80                     | 0.63              |
| 40:RU:34:LYS:HA    | 40:RU:34:LYS:CE   | 2.29                     | 0.63              |
| 47:R1:76:ARG:HD2   | 47:R1:76:ARG:H    | 1.64                     | 0.63              |
| 48:R2:65:ASN:HB3   | 48:R2:69:ARG:NH1  | 2.10                     | 0.63              |
| 54:R8:52:LYS:O     | 54:R8:52:LYS:HG3  | 1.97                     | 0.63              |
| 1:XA:674:G:H2'     | 1:XA:675:A:H8     | 1.62                     | 0.63              |
| 1:XA:1104:G:H4'    | 2:XB:111:ARG:NH1  | 2.14                     | 0.63              |
| 2:XB:37:ASN:C      | 2:XB:39:ILE:H     | 2.07                     | 0.63              |
| 2:XB:214:ILE:HD13  | 2:XB:217:ARG:NH2  | 2.14                     | 0.63              |
| 4:XD:153:ARG:HD3   | 4:XD:181:MET:SD   | 2.39                     | 0.63              |
| 5:XE:51:VAL:O      | 5:XE:55:VAL:HG23  | 1.99                     | 0.63              |
| 9:XI:17:VAL:HG21   | 9:XI:81:ILE:N     | 2.14                     | 0.63              |
| 14:YN:18:VAL:HG23  | 14:YN:19:ARG:N    | 2.14                     | 0.63              |
| 14:YN:42:ILE:C     | 14:YN:43:CYS:O    | 2.41                     | 0.63              |
| 22:XV:6:G:H1       | 22:XV:67:C:H42    | 1.45                     | 0.63              |
| 28:YE:4:ILE:CD1    | 28:YE:28:ALA:HB1  | 2.29                     | 0.63              |
| 28:YE:13:ARG:HH12  | 28:YE:21:VAL:HG12 | 1.64                     | 0.63              |
| 30:YG:61:ALA:HB2   | 30:YG:68:PRO:HD2  | 1.81                     | 0.63              |
| 31:YH:86:GLU:O     | 31:YH:87:LEU:HB2  | 1.99                     | 0.63              |
| 33:YN:87:LEU:O     | 33:YN:87:LEU:HD23 | 1.99                     | 0.63              |
| 35:YP:1:MET:CE     | 35:YP:5:ASP:HB3   | 2.24                     | 0.63              |
| 35:YP:64:LYS:HB2   | 54:Y8:25:MET:HG3  | 1.81                     | 0.63              |
| 39:YT:49:VAL:HG13  | 39:YT:49:VAL:O    | 1.99                     | 0.63              |
| 42:YW:74:ALA:O     | 42:YW:75:TYR:HB3  | 1.98                     | 0.63              |
| 47:Y1:18:ILE:HG12  | 47:Y1:37:ILE:HG12 | 1.81                     | 0.63              |
| 2:QB:21:ARG:HB2    | 2:QB:39:ILE:HA    | 1.80                     | 0.62              |
| 11:QK:12:ARG:HG2   | 11:QK:13:GLN:N    | 2.14                     | 0.62              |
| 25:RA:1678:G:H22   | 25:RA:1989:G:H22  | 1.47                     | 0.62              |
| 27:RD:44:ASN:HB3   | 27:RD:49:ILE:CA   | 2.27                     | 0.62              |
| 29:RF:119:ARG:HH11 | 29:RF:119:ARG:HG2 | 1.64                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:136:ILE:H   | 31:RH:136:ILE:HD12 | 1.64                     | 0.62              |
| 34:RO:8:LEU:HB2   | 34:RO:19:ILE:HD11  | 1.81                     | 0.62              |
| 37:RR:2:ARG:HG2   | 37:RR:5:LYS:HZ1    | 1.63                     | 0.62              |
| 37:RR:117:VAL:O   | 37:RR:118:GLU:HB3  | 1.99                     | 0.62              |
| 44:RY:86:ARG:O    | 44:RY:92:ASN:HB2   | 1.97                     | 0.62              |
| 48:R2:46:GLN:HA   | 48:R2:46:GLN:OE1   | 1.98                     | 0.62              |
| 2:XB:236:TYR:CD2  | 2:XB:239:VAL:HG21  | 2.34                     | 0.62              |
| 4:XD:163:GLU:C    | 4:XD:165:MET:H     | 2.03                     | 0.62              |
| 5:XE:91:LEU:HA    | 5:XE:120:THR:HG22  | 1.81                     | 0.62              |
| 6:XF:62:TRP:C     | 6:XF:63:TYR:HD2    | 2.06                     | 0.62              |
| 9:XI:47:LEU:HD22  | 9:XI:47:LEU:N      | 2.14                     | 0.62              |
| 25:YA:2361:A:O5'  | 54:Y8:27:THR:OG1   | 2.16                     | 0.62              |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA3  | 1.81                     | 0.62              |
| 36:YQ:10:ARG:O    | 36:YQ:11:LYS:HB2   | 1.98                     | 0.62              |
| 44:YY:87:LYS:O    | 44:YY:88:LYS:NZ    | 2.32                     | 0.62              |
| 2:QB:23:ARG:HD3   | 2:QB:23:ARG:H      | 1.64                     | 0.62              |
| 2:QB:66:GLY:O     | 2:QB:67:THR:HG23   | 2.00                     | 0.62              |
| 2:QB:236:TYR:CD2  | 2:QB:239:VAL:HG21  | 2.34                     | 0.62              |
| 5:QE:51:VAL:O     | 5:QE:55:VAL:HG23   | 1.99                     | 0.62              |
| 8:QH:42:GLU:HG3   | 8:QH:109:ILE:HD12  | 1.80                     | 0.62              |
| 9:QI:118:LYS:O    | 9:QI:119:ALA:HB3   | 1.99                     | 0.62              |
| 11:QK:58:PRO:HD3  | 11:QK:89:ALA:HB1   | 1.81                     | 0.62              |
| 18:QR:82:THR:HG22 | 18:QR:83:GLU:N     | 2.15                     | 0.62              |
| 25:RA:517:C:O2'   | 42:RW:18:ARG:NH2   | 2.32                     | 0.62              |
| 25:RA:565:C:OP1   | 41:RV:82:ARG:NH2   | 2.32                     | 0.62              |
| 25:RA:1332:G:H21  | 25:RA:1610:A:H8    | 1.47                     | 0.62              |
| 25:RA:1918:A:O2'  | 25:RA:1920:C:N4    | 2.31                     | 0.62              |
| 29:RF:28:ILE:HD13 | 29:RF:30:PRO:HD3   | 1.80                     | 0.62              |
| 33:RN:101:HIS:ND1 | 33:RN:101:HIS:C    | 2.56                     | 0.62              |
| 36:RQ:20:ALA:HB1  | 36:RQ:99:PRO:CD    | 2.29                     | 0.62              |
| 39:RT:24:PRO:O    | 39:RT:94:ALA:HB2   | 2.00                     | 0.62              |
| 52:R6:13:CYS:HB2  | 52:R6:22:ALA:HB3   | 1.81                     | 0.62              |
| 1:XA:842:C:O2'    | 1:XA:848:C:N4      | 2.32                     | 0.62              |
| 3:XC:34:LEU:CD2   | 3:XC:38:ARG:HD2    | 2.29                     | 0.62              |
| 8:XH:16:ALA:HB2   | 8:XH:24:THR:HG21   | 1.81                     | 0.62              |
| 25:YA:2105:C:H2'  | 25:YA:2106:G:H8    | 1.64                     | 0.62              |
| 40:YU:34:LYS:HA   | 40:YU:34:LYS:CE    | 2.29                     | 0.62              |
| 4:QD:165:MET:HE1  | 4:QD:168:ARG:HD2   | 1.81                     | 0.62              |
| 7:QG:140:ASP:HA   | 7:QG:143:ARG:NH1   | 2.14                     | 0.62              |
| 9:QI:17:VAL:HG21  | 9:QI:81:ILE:N      | 2.14                     | 0.62              |
| 25:RA:2287:A:H62  | 25:RA:2344:U:H3    | 1.47                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:RG:94:LEU:HD23  | 30:RG:94:LEU:N    | 2.14                     | 0.62              |
| 36:RQ:90:VAL:C     | 36:RQ:92:GLY:H    | 2.07                     | 0.62              |
| 38:RS:48:LEU:N     | 38:RS:48:LEU:HD12 | 2.14                     | 0.62              |
| 39:RT:96:ARG:NH1   | 39:RT:96:ARG:HB2  | 2.14                     | 0.62              |
| 42:RW:1:MET:HB3    | 42:RW:64:MET:HE3  | 1.81                     | 0.62              |
| 1:XA:192:U:H4'     | 20:XT:102:GLY:O   | 1.99                     | 0.62              |
| 3:XC:3:ASN:HD22    | 3:XC:3:ASN:N      | 1.97                     | 0.62              |
| 7:XG:9:VAL:CG1     | 7:XG:94:ARG:HE    | 2.12                     | 0.62              |
| 8:XH:112:LEU:O     | 8:XH:112:LEU:HD12 | 1.98                     | 0.62              |
| 11:XK:99:GLN:HG2   | 11:XK:105:VAL:CG2 | 2.29                     | 0.62              |
| 25:YA:742:G:H2'    | 25:YA:743:G:C8    | 2.34                     | 0.62              |
| 25:YA:2227:A:H5''  | 27:YD:263:ARG:NH1 | 2.15                     | 0.62              |
| 25:YA:2470:G:H5'   | 36:YQ:56:ARG:HH22 | 1.63                     | 0.62              |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:N   | 2.14                     | 0.62              |
| 30:YG:94:LEU:H     | 30:YG:94:LEU:HD23 | 1.64                     | 0.62              |
| 43:YX:31:HIS:CE1   | 43:YX:33:LYS:HB2  | 2.34                     | 0.62              |
| 43:YX:49:VAL:HG13  | 43:YX:83:VAL:HG13 | 1.80                     | 0.62              |
| 45:YZ:19:ARG:NH1   | 45:YZ:84:GLU:O    | 2.32                     | 0.62              |
| 46:Y0:10:THR:HG22  | 46:Y0:12:ASN:H    | 1.64                     | 0.62              |
| 2:QB:214:ILE:HD13  | 2:QB:217:ARG:NH2  | 2.14                     | 0.62              |
| 5:QE:50:GLU:HG3    | 5:QE:52:PRO:HD2   | 1.79                     | 0.62              |
| 6:QF:8:ILE:HD11    | 6:QF:79:LEU:HD13  | 1.81                     | 0.62              |
| 17:QQ:11:VAL:HG23  | 17:QQ:20:THR:HB   | 1.79                     | 0.62              |
| 25:RA:2784:C:H5''  | 28:RE:41:LYS:HZ3  | 1.64                     | 0.62              |
| 27:RD:72:LYS:HG2   | 27:RD:103:ARG:NH2 | 2.13                     | 0.62              |
| 30:RG:53:LEU:C     | 30:RG:53:LEU:HD23 | 2.25                     | 0.62              |
| 38:RS:22:GLY:O     | 38:RS:23:ARG:O    | 2.17                     | 0.62              |
| 52:R6:41:PRO:HG2   | 52:R6:45:LYS:N    | 2.10                     | 0.62              |
| 1:XA:1014:A:H4'    | 19:XS:14:HIS:NE2  | 2.13                     | 0.62              |
| 4:XD:170:VAL:HG22  | 4:XD:171:GLY:N    | 2.12                     | 0.62              |
| 7:XG:140:ASP:HA    | 7:XG:143:ARG:NH1  | 2.14                     | 0.62              |
| 11:XK:17:GLY:HA3   | 11:XK:77:MET:CE   | 2.21                     | 0.62              |
| 16:XP:51:VAL:CG1   | 16:XP:52:ASP:H    | 2.10                     | 0.62              |
| 25:YA:2277:G:H5'   | 36:YQ:85:LYS:HG3  | 1.80                     | 0.62              |
| 27:YD:35:LYS:HA    | 27:YD:64:ILE:HG22 | 1.81                     | 0.62              |
| 29:YF:129:PHE:O    | 29:YF:130:ALA:HB3 | 2.00                     | 0.62              |
| 33:YN:26:LEU:O     | 33:YN:30:ILE:HG13 | 1.99                     | 0.62              |
| 35:YP:105:LEU:O    | 35:YP:106:LEU:CB  | 2.42                     | 0.62              |
| 38:YS:48:LEU:HD12  | 38:YS:48:LEU:N    | 2.14                     | 0.62              |
| 39:YT:22:PHE:N     | 39:YT:22:PHE:HD2  | 1.97                     | 0.62              |
| 39:YT:96:ARG:NH1   | 39:YT:96:ARG:HB2  | 2.14                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:YX:63:LYS:O    | 43:YX:64:LYS:HD2   | 1.98                     | 0.62              |
| 48:Y2:41:ILE:HG12 | 48:Y2:44:LEU:HD12  | 1.82                     | 0.62              |
| 4:QD:153:ARG:HD3  | 4:QD:181:MET:SD    | 2.39                     | 0.62              |
| 8:QH:84:ARG:HG3   | 8:QH:84:ARG:NH1    | 2.10                     | 0.62              |
| 9:QI:13:ALA:HB2   | 9:QI:67:GLY:O      | 2.00                     | 0.62              |
| 27:RD:134:ARG:HD3 | 27:RD:135:PHE:CE2  | 2.34                     | 0.62              |
| 28:RE:13:ARG:HH12 | 28:RE:21:VAL:HG12  | 1.64                     | 0.62              |
| 29:RF:32:LEU:CD1  | 29:RF:105:VAL:HG13 | 2.29                     | 0.62              |
| 30:RG:77:ILE:HD13 | 30:RG:82:LEU:CD1   | 2.29                     | 0.62              |
| 31:RH:137:ASP:HB3 | 31:RH:140:LYS:HB2  | 1.81                     | 0.62              |
| 35:RP:65:ARG:HH11 | 35:RP:65:ARG:CG    | 2.06                     | 0.62              |
| 43:RX:31:HIS:CE1  | 43:RX:33:LYS:HB2   | 2.34                     | 0.62              |
| 50:R4:38:LYS:C    | 50:R4:40:HIS:N     | 2.52                     | 0.62              |
| 1:XA:188:U:H2'    | 1:XA:189:U:H5''    | 1.82                     | 0.62              |
| 11:XK:57:THR:HG22 | 11:XK:59:TYR:H     | 1.65                     | 0.62              |
| 11:XK:58:PRO:HD3  | 11:XK:89:ALA:HB1   | 1.81                     | 0.62              |
| 18:XR:82:THR:HG22 | 18:XR:83:GLU:N     | 2.15                     | 0.62              |
| 19:XS:5:LEU:HD21  | 50:Y4:66:SER:HB2   | 1.82                     | 0.62              |
| 25:YA:222:A:H62   | 25:YA:232:G:H21    | 1.47                     | 0.62              |
| 25:YA:275:G:H21   | 25:YA:276:A:H62    | 1.47                     | 0.62              |
| 25:YA:1693:U:H1'  | 27:YD:14:ARG:HH22  | 1.65                     | 0.62              |
| 25:YA:2635:C:H5'' | 28:YE:78:LEU:HA    | 1.80                     | 0.62              |
| 30:YG:94:LEU:HD23 | 30:YG:94:LEU:N     | 2.14                     | 0.62              |
| 35:YP:65:ARG:HE   | 54:Y8:15:LYS:HB2   | 1.64                     | 0.62              |
| 37:YR:63:ARG:NH1  | 37:YR:80:PHE:CD1   | 2.67                     | 0.62              |
| 41:YV:52:VAL:CG2  | 41:YV:55:ALA:HB3   | 2.28                     | 0.62              |
| 1:QA:335:C:O2'    | 1:QA:1433:A:N3     | 2.30                     | 0.62              |
| 2:QB:178:ARG:HD2  | 8:QH:71:GLY:HA2    | 1.81                     | 0.62              |
| 4:QD:106:TYR:HE1  | 4:QD:112:VAL:O     | 1.82                     | 0.62              |
| 9:QI:65:VAL:HG21  | 9:QI:73:GLN:HB3    | 1.81                     | 0.62              |
| 14:QN:41:ARG:HH21 | 14:QN:42:ILE:HD11  | 1.62                     | 0.62              |
| 15:QO:26:GLU:CD   | 15:QO:77:ARG:NH1   | 2.58                     | 0.62              |
| 25:RA:392:C:H5''  | 25:RA:409:C:H5''   | 1.82                     | 0.62              |
| 28:RE:35:GLN:CG   | 28:RE:37:ARG:NE    | 2.62                     | 0.62              |
| 33:RN:87:LEU:O    | 33:RN:87:LEU:HD23  | 1.99                     | 0.62              |
| 33:RN:96:GLU:O    | 33:RN:98:VAL:N     | 2.33                     | 0.62              |
| 35:RP:61:ARG:H    | 35:RP:61:ARG:CD    | 2.09                     | 0.62              |
| 35:RP:83:VAL:HG12 | 35:RP:112:LEU:HD21 | 1.81                     | 0.62              |
| 39:RT:108:ARG:O   | 39:RT:111:ARG:HG3  | 2.00                     | 0.62              |
| 44:RY:87:LYS:O    | 44:RY:88:LYS:NZ    | 2.31                     | 0.62              |
| 47:R1:18:ILE:HG12 | 47:R1:37:ILE:HG12  | 1.81                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:XB:20:GLU:HB2    | 2:XB:190:THR:OG1   | 1.99                     | 0.62              |
| 2:XB:23:ARG:HD3    | 2:XB:23:ARG:H      | 1.64                     | 0.62              |
| 2:XB:115:LEU:CD2   | 2:XB:153:ARG:HD3   | 2.30                     | 0.62              |
| 8:XH:58:TYR:O      | 8:XH:59:LEU:HD23   | 2.00                     | 0.62              |
| 10:XJ:29:ARG:HG2   | 10:XJ:29:ARG:O     | 2.00                     | 0.62              |
| 14:XN:53:LEU:HB3   | 14:XN:56:VAL:HG21  | 1.80                     | 0.62              |
| 25:YA:2445:G:OP1   | 29:YF:74:ARG:NH2   | 2.32                     | 0.62              |
| 28:YE:131:ALA:HB1  | 28:YE:135:HIS:CE1  | 2.34                     | 0.62              |
| 31:YH:136:ILE:HD12 | 31:YH:136:ILE:H    | 1.64                     | 0.62              |
| 35:YP:112:LEU:HD11 | 35:YP:114:ILE:HG23 | 1.80                     | 0.62              |
| 39:YT:108:ARG:O    | 39:YT:111:ARG:HG3  | 2.00                     | 0.62              |
| 44:YY:48:ALA:HB2   | 44:YY:61:ILE:HD13  | 1.82                     | 0.62              |
| 48:Y2:40:SER:C     | 48:Y2:42:GLY:N     | 2.51                     | 0.62              |
| 48:Y2:69:ARG:HB2   | 48:Y2:69:ARG:CZ    | 2.29                     | 0.62              |
| 48:Y2:70:GLN:O     | 48:Y2:71:ASN:HB2   | 2.00                     | 0.62              |
| 52:Y6:13:CYS:HB2   | 52:Y6:22:ALA:HB3   | 1.81                     | 0.62              |
| 9:QI:62:TYR:O      | 9:QI:63:ILE:HD12   | 1.98                     | 0.62              |
| 9:QI:116:LYS:O     | 9:QI:118:LYS:N     | 2.33                     | 0.62              |
| 13:QM:97:PRO:HB2   | 13:QM:101:GLN:HE22 | 1.65                     | 0.62              |
| 30:RG:68:PRO:HB2   | 30:RG:90:LEU:HD12  | 1.80                     | 0.62              |
| 41:RV:36:PRO:HA    | 41:RV:56:SER:OG    | 1.99                     | 0.62              |
| 2:XB:194:PRO:HG2   | 2:XB:195:ASP:H     | 1.64                     | 0.62              |
| 4:XD:96:LEU:H      | 4:XD:96:LEU:CD2    | 2.11                     | 0.62              |
| 11:XK:51:LYS:CA    | 11:XK:55:LYS:HD3   | 2.22                     | 0.62              |
| 25:YA:898:C:H2'    | 25:YA:899:A:H5'    | 1.82                     | 0.62              |
| 30:YG:170:ARG:O    | 30:YG:174:GLU:HB2  | 1.99                     | 0.62              |
| 38:YS:100:ALA:HA   | 38:YS:103:GLU:CG   | 2.30                     | 0.62              |
| 42:YW:1:MET:HB3    | 42:YW:64:MET:HE3   | 1.82                     | 0.62              |
| 50:Y4:61:ARG:O     | 50:Y4:63:TYR:N     | 2.33                     | 0.62              |
| 1:QA:579:G:H5'     | 1:QA:728:A:H1'     | 1.82                     | 0.62              |
| 11:QK:57:THR:HG22  | 11:QK:59:TYR:H     | 1.64                     | 0.62              |
| 13:QM:66:LEU:HA    | 13:QM:70:LEU:HD23  | 1.81                     | 0.62              |
| 14:QN:23:ARG:NH1   | 14:QN:30:ALA:HB2   | 2.14                     | 0.62              |
| 27:RD:137:PRO:HB2  | 27:RD:140:THR:HG23 | 1.81                     | 0.62              |
| 33:RN:26:LEU:O     | 33:RN:30:ILE:HG13  | 1.99                     | 0.62              |
| 35:RP:64:LYS:HB2   | 54:R8:25:MET:HG3   | 1.80                     | 0.62              |
| 39:RT:57:PHE:CD2   | 39:RT:58:ASN:N     | 2.66                     | 0.62              |
| 48:R2:69:ARG:HB2   | 48:R2:69:ARG:CZ    | 2.30                     | 0.62              |
| 13:XM:66:LEU:HA    | 13:XM:70:LEU:HD23  | 1.81                     | 0.62              |
| 13:XM:69:GLU:O     | 13:XM:72:ALA:N     | 2.32                     | 0.62              |
| 19:XS:12:ASP:OD1   | 19:XS:37:ARG:HD2   | 2.00                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:XS:39:THR:HG22  | 19:XS:40:ILE:N     | 2.14                     | 0.62              |
| 20:XT:14:LYS:HA    | 20:XT:17:ARG:NH1   | 2.14                     | 0.62              |
| 22:XV:76:A:O2'     | 56:Z8:76:PPU:N     | 2.28                     | 0.62              |
| 25:YA:1697:G:O2'   | 25:YA:1978:A:OP1   | 2.16                     | 0.62              |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:CB   | 2.29                     | 0.62              |
| 27:YD:134:ARG:HD3  | 27:YD:135:PHE:CE2  | 2.35                     | 0.62              |
| 29:YF:28:ILE:HD13  | 29:YF:30:PRO:HD3   | 1.80                     | 0.62              |
| 30:YG:53:LEU:C     | 30:YG:53:LEU:HD23  | 2.24                     | 0.62              |
| 34:YO:104:ARG:CZ   | 39:YT:34:VAL:HG11  | 2.29                     | 0.62              |
| 35:YP:50:ARG:CB    | 35:YP:50:ARG:NH2   | 2.58                     | 0.62              |
| 37:YR:79:LEU:HD23  | 37:YR:79:LEU:C     | 2.23                     | 0.62              |
| 42:YW:86:LEU:HD12  | 42:YW:87:PRO:CD    | 2.23                     | 0.62              |
| 1:QA:243:A:N6      | 1:QA:281:G:O2'     | 2.33                     | 0.62              |
| 1:QA:395:C:H4'     | 32:YI:118:LYS:HE2  | 1.81                     | 0.62              |
| 1:QA:1226:C:OP2    | 13:QM:103:THR:OG1  | 2.12                     | 0.62              |
| 3:QC:127:ARG:HH11  | 3:QC:127:ARG:HG2   | 1.64                     | 0.62              |
| 6:QF:10:LEU:HD13   | 6:QF:61:LEU:CD1    | 2.30                     | 0.62              |
| 10:QJ:22:LYS:HD2   | 10:QJ:22:LYS:C     | 2.25                     | 0.62              |
| 11:QK:17:GLY:HA3   | 11:QK:77:MET:CE    | 2.20                     | 0.62              |
| 18:QR:25:THR:HG22  | 18:QR:25:THR:O     | 2.00                     | 0.62              |
| 27:RD:27:THR:O     | 27:RD:29:PRO:HD2   | 1.99                     | 0.62              |
| 27:RD:70:TRP:CH2   | 27:RD:150:LYS:HA   | 2.35                     | 0.62              |
| 27:RD:72:LYS:HE3   | 27:RD:75:ILE:HD12  | 1.82                     | 0.62              |
| 28:RE:35:GLN:HG2   | 28:RE:37:ARG:NE    | 2.14                     | 0.62              |
| 29:RF:129:PHE:O    | 29:RF:130:ALA:HB3  | 2.00                     | 0.62              |
| 30:RG:6:ALA:HB2    | 50:R4:23:GLU:OE2   | 2.00                     | 0.62              |
| 30:RG:9:ARG:HG2    | 30:RG:13:GLU:OE1   | 2.00                     | 0.62              |
| 38:RS:26:LEU:HD22  | 38:RS:87:PHE:HD1   | 1.64                     | 0.62              |
| 39:RT:22:PHE:N     | 39:RT:22:PHE:HD2   | 1.97                     | 0.62              |
| 47:R1:81:LYS:NZ    | 47:R1:81:LYS:CA    | 2.31                     | 0.62              |
| 47:R1:91:LYS:HA    | 47:R1:91:LYS:HE3   | 1.82                     | 0.62              |
| 48:R2:17:SER:HB2   | 48:R2:18:PRO:CA    | 2.30                     | 0.62              |
| 50:R4:61:ARG:O     | 50:R4:63:TYR:N     | 2.33                     | 0.62              |
| 52:R6:18:ARG:O     | 52:R6:18:ARG:HD2   | 2.00                     | 0.62              |
| 54:R8:33:ASN:O     | 54:R8:34:TRP:C     | 2.42                     | 0.62              |
| 3:XC:111:LEU:HD21  | 3:XC:144:SER:O     | 2.00                     | 0.62              |
| 9:XI:116:LYS:O     | 9:XI:118:LYS:N     | 2.33                     | 0.62              |
| 17:XQ:65:ILE:HD12  | 17:XQ:65:ILE:N     | 2.15                     | 0.62              |
| 25:YA:1803:A:H4'   | 27:YD:259:THR:HG21 | 1.82                     | 0.62              |
| 29:YF:28:ILE:HG22  | 29:YF:112:MET:HB3  | 1.80                     | 0.62              |
| 34:YO:7:TYR:HE1    | 34:YO:20:MET:HE3   | 1.65                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:121:HIS:ND1  | 45:YZ:123:ASP:O    | 2.32                     | 0.62              |
| 47:Y1:91:LYS:HA    | 47:Y1:91:LYS:HE3   | 1.82                     | 0.62              |
| 1:QA:411:A:C5      | 1:QA:413:G:H1'     | 2.35                     | 0.62              |
| 4:QD:13:ARG:HB2    | 4:QD:33:MET:HE3    | 1.82                     | 0.62              |
| 5:QE:51:VAL:HB     | 5:QE:52:PRO:CD     | 2.30                     | 0.62              |
| 5:QE:148:VAL:HG21  | 8:QH:107:LEU:HD13  | 1.82                     | 0.62              |
| 6:QF:77:ARG:HB2    | 6:QF:77:ARG:NH1    | 2.15                     | 0.62              |
| 8:QH:16:ALA:HB2    | 8:QH:24:THR:HG21   | 1.82                     | 0.62              |
| 13:QM:117:VAL:HG22 | 13:QM:118:ALA:N    | 2.15                     | 0.62              |
| 14:QN:44:LEU:C     | 14:QN:44:LEU:HD12  | 2.24                     | 0.62              |
| 15:QO:76:GLU:C     | 15:QO:78:TYR:H     | 2.08                     | 0.62              |
| 19:QS:69:HIS:CE1   | 50:R4:69:LYS:CE    | 2.81                     | 0.62              |
| 25:RA:297:C:H5''   | 44:RY:85:VAL:HG21  | 1.82                     | 0.62              |
| 25:RA:1937:A:N7    | 25:RA:1939:U:H2'   | 2.15                     | 0.62              |
| 30:RG:111:LEU:HB2  | 30:RG:112:PRO:HD3  | 1.82                     | 0.62              |
| 34:RO:78:ARG:HH21  | 39:RT:103:ARG:NH2  | 1.98                     | 0.62              |
| 35:RP:114:ILE:HD11 | 35:RP:130:PHE:CD1  | 2.34                     | 0.62              |
| 38:RS:26:LEU:HD12  | 38:RS:39:ILE:CD1   | 2.23                     | 0.62              |
| 44:RY:101:LYS:HE3  | 44:RY:102:CYS:SG   | 2.40                     | 0.62              |
| 52:R6:44:ARG:O     | 52:R6:45:LYS:HB2   | 2.00                     | 0.62              |
| 1:XA:1376:U:H2'    | 1:XA:1377:A:C8     | 2.35                     | 0.62              |
| 3:XC:189:ALA:O     | 3:XC:191:THR:HG23  | 1.99                     | 0.62              |
| 5:XE:51:VAL:HB     | 5:XE:52:PRO:CD     | 2.30                     | 0.62              |
| 9:XI:65:VAL:HG21   | 9:XI:73:GLN:HB3    | 1.81                     | 0.62              |
| 15:XO:26:GLU:CD    | 15:XO:77:ARG:NH1   | 2.58                     | 0.62              |
| 16:XP:4:ILE:HG13   | 16:XP:21:VAL:CG1   | 2.29                     | 0.62              |
| 16:XP:20:VAL:HG21  | 16:XP:32:TYR:CD2   | 2.35                     | 0.62              |
| 25:YA:528:A:C2     | 25:YA:2042:A:H2'   | 2.35                     | 0.62              |
| 25:YA:643:A:N1     | 25:YA:2369:A:O2'   | 2.29                     | 0.62              |
| 25:YA:888:C:H3'    | 25:YA:889:C:H4'    | 1.82                     | 0.62              |
| 25:YA:2438:U:O3'   | 25:YA:2439:A:H3'   | 1.99                     | 0.62              |
| 30:YG:112:PRO:HB3  | 50:Y4:37:SER:CB    | 2.25                     | 0.62              |
| 32:YI:92:VAL:HG13  | 32:YI:120:ILE:HG23 | 1.80                     | 0.62              |
| 34:YO:1:MET:HE3    | 34:YO:67:LYS:HE2   | 1.82                     | 0.62              |
| 1:QA:977:A:O2'     | 1:QA:981:U:N3      | 2.32                     | 0.61              |
| 7:QG:15:ASP:O      | 7:QG:19:GLY:HA2    | 2.00                     | 0.61              |
| 8:QH:29:SER:HB3    | 8:QH:32:LYS:CG     | 2.22                     | 0.61              |
| 13:QM:69:GLU:O     | 13:QM:72:ALA:N     | 2.32                     | 0.61              |
| 14:QN:18:VAL:HG23  | 14:QN:19:ARG:N     | 2.14                     | 0.61              |
| 15:QO:68:ARG:O     | 15:QO:72:ARG:HB2   | 2.00                     | 0.61              |
| 30:RG:170:ARG:O    | 30:RG:174:GLU:HB2  | 2.00                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:RN:7:LYS:HD2    | 33:RN:7:LYS:H      | 1.64                     | 0.61              |
| 35:RP:50:ARG:CB    | 35:RP:50:ARG:NH2   | 2.57                     | 0.61              |
| 38:RS:100:ALA:HA   | 38:RS:103:GLU:CG   | 2.30                     | 0.61              |
| 39:RT:31:SER:HA    | 39:RT:44:ASP:OD2   | 2.00                     | 0.61              |
| 3:XC:127:ARG:HH11  | 3:XC:127:ARG:HG2   | 1.64                     | 0.61              |
| 6:XF:8:ILE:HD11    | 6:XF:79:LEU:HD13   | 1.81                     | 0.61              |
| 9:XI:59:PHE:HZ     | 9:XI:88:TYR:CE1    | 2.17                     | 0.61              |
| 25:YA:593:G:O3'    | 54:Y8:61:LEU:HD22  | 2.00                     | 0.61              |
| 25:YA:2392:A:H2    | 25:YA:2424:C:H42   | 1.46                     | 0.61              |
| 27:YD:182:LEU:H    | 27:YD:272:ALA:HB3  | 1.63                     | 0.61              |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:HG23 | 1.82                     | 0.61              |
| 30:YG:142:PRO:HB2  | 50:Y4:31:ILE:CD1   | 2.30                     | 0.61              |
| 33:YN:133:GLN:O    | 33:YN:134:ARG:HB3  | 1.99                     | 0.61              |
| 40:YU:102:GLU:HG3  | 41:YV:2:PHE:CE2    | 2.34                     | 0.61              |
| 47:Y1:76:ARG:HD2   | 47:Y1:76:ARG:H     | 1.64                     | 0.61              |
| 48:Y2:17:SER:HB2   | 48:Y2:18:PRO:CA    | 2.30                     | 0.61              |
| 1:QA:565:U:H5''    | 1:QA:566:G:H2'     | 1.82                     | 0.61              |
| 2:QB:108:ILE:O     | 2:QB:111:ARG:HB2   | 2.00                     | 0.61              |
| 3:QC:111:LEU:HD21  | 3:QC:144:SER:O     | 2.01                     | 0.61              |
| 10:QJ:53:PRO:HA    | 14:QN:42:ILE:HD12  | 1.82                     | 0.61              |
| 19:QS:11:VAL:O     | 19:QS:12:ASP:HB2   | 2.00                     | 0.61              |
| 27:RD:133:LEU:HD21 | 27:RD:191:ALA:HB2  | 1.82                     | 0.61              |
| 27:RD:237:GLU:OE1  | 27:RD:237:GLU:CA   | 2.48                     | 0.61              |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:N    | 2.07                     | 0.61              |
| 34:RO:1:MET:HE3    | 34:RO:67:LYS:HE2   | 1.82                     | 0.61              |
| 34:RO:97:ARG:N     | 34:RO:117:LEU:HD22 | 2.15                     | 0.61              |
| 1:XA:1002:G:H2'    | 1:XA:1003:G:H8     | 1.65                     | 0.61              |
| 1:XA:1004:A:O5'    | 1:XA:1025:U:N3     | 2.33                     | 0.61              |
| 4:XD:149:ALA:HB3   | 4:XD:152:SER:HB2   | 1.82                     | 0.61              |
| 5:XE:111:GLU:C     | 5:XE:113:ALA:H     | 2.07                     | 0.61              |
| 25:YA:928:G:O2'    | 49:Y3:43:ILE:HD11  | 2.00                     | 0.61              |
| 25:YA:1062:G:H2'   | 25:YA:1063:G:C8    | 2.36                     | 0.61              |
| 25:YA:2758:A:C4    | 31:YH:67:LEU:HD21  | 2.35                     | 0.61              |
| 27:YD:35:LYS:HZ1   | 27:YD:65:ILE:HA    | 1.65                     | 0.61              |
| 35:YP:108:LYS:HD2  | 35:YP:108:LYS:H    | 1.64                     | 0.61              |
| 39:YT:105:LEU:C    | 39:YT:107:ASP:H    | 2.08                     | 0.61              |
| 40:YU:79:PHE:CD2   | 40:YU:79:PHE:C     | 2.78                     | 0.61              |
| 44:YY:44:ILE:HG13  | 44:YY:45:VAL:H     | 1.64                     | 0.61              |
| 53:Y7:31:LEU:O     | 53:Y7:32:LYS:C     | 2.43                     | 0.61              |
| 6:QF:97:PHE:C      | 6:QF:97:PHE:CD2    | 2.76                     | 0.61              |
| 11:QK:121:PRO:HD2  | 11:QK:126:ARG:HD3  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:QP:66:PRO:HG2  | 16:QP:71:ARG:HH12  | 1.64                     | 0.61              |
| 18:QR:57:GLY:O    | 18:QR:58:LEU:C     | 2.44                     | 0.61              |
| 25:RA:259:G:H21   | 25:RA:621:A:H8     | 1.46                     | 0.61              |
| 25:RA:2633:G:H1'  | 28:RE:62:PRO:HG2   | 1.81                     | 0.61              |
| 27:RD:230:ASP:O   | 27:RD:231:HIS:HB2  | 1.99                     | 0.61              |
| 30:RG:112:PRO:HB3 | 50:R4:37:SER:CB    | 2.26                     | 0.61              |
| 31:RH:152:ARG:O   | 31:RH:153:LYS:CD   | 2.48                     | 0.61              |
| 37:RR:38:VAL:HB   | 37:RR:39:PRO:HD3   | 1.81                     | 0.61              |
| 39:RT:105:LEU:C   | 39:RT:107:ASP:H    | 2.08                     | 0.61              |
| 40:RU:92:ARG:HD3  | 40:RU:94:ASN:HB3   | 1.82                     | 0.61              |
| 50:R4:23:GLU:O    | 50:R4:25:TYR:N     | 2.33                     | 0.61              |
| 50:R4:71:ARG:NH1  | 50:R4:71:ARG:CG    | 2.61                     | 0.61              |
| 54:R8:59:LYS:HZ3  | 54:R8:59:LYS:HB3   | 1.65                     | 0.61              |
| 1:XA:489:C:OP1    | 4:XD:132:ARG:NH2   | 2.33                     | 0.61              |
| 6:XF:77:ARG:HB2   | 6:XF:77:ARG:NH1    | 2.15                     | 0.61              |
| 21:XU:15:ARG:HH11 | 21:XU:15:ARG:HG2   | 1.63                     | 0.61              |
| 25:YA:1153:C:OP1  | 40:YU:76:TYR:OH    | 2.18                     | 0.61              |
| 25:YA:1472:A:H3'  | 25:YA:1473:G:H5''  | 1.81                     | 0.61              |
| 29:YF:32:LEU:CD1  | 29:YF:105:VAL:HG13 | 2.29                     | 0.61              |
| 34:YO:8:LEU:HB2   | 34:YO:19:ILE:HD11  | 1.81                     | 0.61              |
| 42:YW:5:ALA:O     | 42:YW:50:VAL:HG13  | 2.00                     | 0.61              |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HA   | 1.82                     | 0.61              |
| 50:Y4:23:GLU:O    | 50:Y4:25:TYR:N     | 2.33                     | 0.61              |
| 1:QA:1002:G:H2'   | 1:QA:1003:G:H8     | 1.65                     | 0.61              |
| 4:QD:129:ASN:HA   | 4:QD:145:GLU:HB2   | 1.82                     | 0.61              |
| 4:QD:166:LYS:HG2  | 27:YD:134:ARG:CZ   | 2.30                     | 0.61              |
| 5:QE:91:LEU:HA    | 5:QE:120:THR:HG22  | 1.81                     | 0.61              |
| 8:QH:39:LEU:O     | 8:QH:45:ILE:HG12   | 2.01                     | 0.61              |
| 12:QL:10:LEU:HD13 | 17:QQ:32:TYR:CD2   | 2.35                     | 0.61              |
| 14:QN:23:ARG:CD   | 14:QN:28:GLY:O     | 2.49                     | 0.61              |
| 25:RA:2815:C:H5'  | 51:R5:29:THR:HG21  | 1.81                     | 0.61              |
| 31:RH:86:GLU:O    | 31:RH:87:LEU:HB2   | 1.99                     | 0.61              |
| 44:RY:48:ALA:HB2  | 44:RY:61:ILE:HD13  | 1.82                     | 0.61              |
| 47:R1:80:LEU:O    | 47:R1:81:LYS:HD2   | 2.01                     | 0.61              |
| 49:R3:29:ARG:HH11 | 49:R3:29:ARG:CB    | 2.13                     | 0.61              |
| 5:XE:131:ILE:O    | 5:XE:134:ALA:HB3   | 2.01                     | 0.61              |
| 7:XG:15:ASP:O     | 7:XG:19:GLY:HA2    | 2.00                     | 0.61              |
| 12:XL:85:ILE:HD11 | 12:XL:98:TYR:HB2   | 1.81                     | 0.61              |
| 15:XO:74:ASP:OD1  | 15:XO:77:ARG:HG2   | 2.00                     | 0.61              |
| 27:YD:27:THR:O    | 27:YD:29:PRO:HD2   | 1.99                     | 0.61              |
| 27:YD:137:PRO:HB2 | 27:YD:140:THR:HG23 | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:YD:227:ASN:CB  | 27:YD:228:PRO:HD2 | 2.24                     | 0.61              |
| 28:YE:35:GLN:HG2  | 28:YE:37:ARG:NE   | 2.14                     | 0.61              |
| 31:YH:6:ARG:HG3   | 31:YH:7:LEU:N     | 2.15                     | 0.61              |
| 31:YH:137:ASP:HB3 | 31:YH:140:LYS:HB2 | 1.81                     | 0.61              |
| 31:YH:152:ARG:O   | 31:YH:153:LYS:CD  | 2.48                     | 0.61              |
| 33:YN:62:VAL:CG1  | 33:YN:66:LYS:HD2  | 2.29                     | 0.61              |
| 36:YQ:54:MET:O    | 36:YQ:57:HIS:HB3  | 2.00                     | 0.61              |
| 36:YQ:66:ILE:CG1  | 36:YQ:67:ARG:H    | 2.12                     | 0.61              |
| 39:YT:24:PRO:O    | 39:YT:94:ALA:HB2  | 2.00                     | 0.61              |
| 39:YT:31:SER:HA   | 39:YT:44:ASP:OD2  | 2.00                     | 0.61              |
| 41:YV:46:VAL:O    | 41:YV:46:VAL:HG13 | 2.01                     | 0.61              |
| 43:YX:15:GLU:N    | 43:YX:15:GLU:OE1  | 2.34                     | 0.61              |
| 44:YY:19:LYS:O    | 44:YY:19:LYS:HG3  | 2.01                     | 0.61              |
| 54:Y8:33:ASN:O    | 54:Y8:34:TRP:C    | 2.42                     | 0.61              |
| 4:QD:11:LEU:HA    | 4:QD:14:ARG:HB2   | 1.82                     | 0.61              |
| 5:QE:42:GLY:HA2   | 5:QE:136:MET:HE1  | 1.82                     | 0.61              |
| 10:QJ:98:ILE:HD12 | 10:QJ:98:ILE:N    | 2.16                     | 0.61              |
| 12:QL:48:PRO:CD   | 12:QL:49:ASN:H    | 2.10                     | 0.61              |
| 16:QP:4:ILE:HG13  | 16:QP:21:VAL:CG1  | 2.29                     | 0.61              |
| 25:RA:307:G:H21   | 25:RA:330:A:H62   | 1.47                     | 0.61              |
| 30:RG:142:PRO:HB2 | 50:R4:31:ILE:CD1  | 2.30                     | 0.61              |
| 35:RP:65:ARG:HE   | 54:R8:15:LYS:HB2  | 1.64                     | 0.61              |
| 38:RS:88:ASP:O    | 38:RS:89:ARG:CB   | 2.49                     | 0.61              |
| 42:RW:5:ALA:O     | 42:RW:50:VAL:HG13 | 2.00                     | 0.61              |
| 50:R4:35:VAL:O    | 50:R4:37:SER:N    | 2.26                     | 0.61              |
| 52:R6:25:LYS:HD2  | 54:R8:34:TRP:CZ2  | 2.36                     | 0.61              |
| 1:XA:1446:A:O2'   | 1:XA:1447:G:O5'   | 2.16                     | 0.61              |
| 6:XF:89:MET:HE1   | 18:XR:76:LEU:HD22 | 1.82                     | 0.61              |
| 9:XI:28:VAL:HG13  | 9:XI:63:ILE:HG22  | 1.83                     | 0.61              |
| 20:XT:34:LYS:O    | 20:XT:38:LYS:HB2  | 2.01                     | 0.61              |
| 27:YD:35:LYS:NZ   | 27:YD:65:ILE:HA   | 2.15                     | 0.61              |
| 28:YE:69:LYS:C    | 28:YE:71:GLY:H    | 2.08                     | 0.61              |
| 28:YE:174:ASP:CG  | 28:YE:175:VAL:N   | 2.58                     | 0.61              |
| 30:YG:6:ALA:HB2   | 50:Y4:23:GLU:OE2  | 1.99                     | 0.61              |
| 33:YN:96:GLU:O    | 33:YN:98:VAL:N    | 2.33                     | 0.61              |
| 36:YQ:2:LEU:HD23  | 36:YQ:2:LEU:H     | 1.65                     | 0.61              |
| 52:Y6:27:LYS:HB2  | 52:Y6:27:LYS:HZ2  | 1.63                     | 0.61              |
| 1:QA:346:G:H1'    | 1:QA:347:G:H5'    | 1.81                     | 0.61              |
| 4:QD:162:LEU:CD1  | 4:QD:181:MET:HB3  | 2.31                     | 0.61              |
| 4:QD:170:VAL:O    | 6:XF:21:LEU:HD21  | 2.01                     | 0.61              |
| 10:QJ:34:VAL:CG2  | 10:QJ:74:ILE:HG22 | 2.30                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:QK:12:ARG:HG2   | 11:QK:13:GLN:H     | 1.64                     | 0.61              |
| 11:QK:99:GLN:HG2   | 11:QK:105:VAL:CG2  | 2.28                     | 0.61              |
| 20:QT:47:GLY:C     | 20:QT:49:ALA:H     | 2.07                     | 0.61              |
| 27:RD:21:PHE:HB3   | 27:RD:24:ILE:HG13  | 1.83                     | 0.61              |
| 27:RD:35:LYS:HA    | 27:RD:64:ILE:HG22  | 1.82                     | 0.61              |
| 27:RD:174:ILE:N    | 27:RD:174:ILE:HD12 | 2.16                     | 0.61              |
| 31:RH:6:ARG:HG3    | 31:RH:7:LEU:N      | 2.15                     | 0.61              |
| 33:RN:62:VAL:CG1   | 33:RN:66:LYS:HD2   | 2.30                     | 0.61              |
| 42:RW:82:LEU:HB2   | 42:RW:98:LYS:HB2   | 1.82                     | 0.61              |
| 43:RX:66:LEU:O     | 43:RX:66:LEU:HD23  | 2.01                     | 0.61              |
| 45:RZ:157:LEU:HD23 | 45:RZ:161:VAL:HG12 | 1.82                     | 0.61              |
| 2:XB:17:PHE:CD2    | 2:XB:44:LEU:HD11   | 2.36                     | 0.61              |
| 2:XB:108:ILE:O     | 2:XB:111:ARG:HB2   | 2.01                     | 0.61              |
| 7:XG:148:ASN:C     | 7:XG:150:ALA:H     | 2.08                     | 0.61              |
| 8:XH:102:ARG:HH11  | 8:XH:105:ARG:NH2   | 1.99                     | 0.61              |
| 27:YD:70:TRP:CH2   | 27:YD:150:LYS:HA   | 2.35                     | 0.61              |
| 27:YD:147:LEU:CD1  | 27:YD:155:LEU:HD11 | 2.26                     | 0.61              |
| 28:YE:35:GLN:CG    | 28:YE:37:ARG:HE    | 2.10                     | 0.61              |
| 28:YE:95:ILE:HD12  | 28:YE:95:ILE:N     | 2.15                     | 0.61              |
| 29:YF:119:ARG:HH11 | 29:YF:119:ARG:HG2  | 1.64                     | 0.61              |
| 40:YU:88:ILE:H     | 40:YU:88:ILE:CD1   | 2.05                     | 0.61              |
| 42:YW:28:SER:O     | 42:YW:31:GLU:N     | 2.34                     | 0.61              |
| 52:Y6:18:ARG:O     | 52:Y6:18:ARG:HD2   | 2.00                     | 0.61              |
| 54:Y8:22:VAL:HG21  | 54:Y8:53:PRO:HB2   | 1.83                     | 0.61              |
| 1:QA:1015:A:N3     | 1:QA:1218:C:O2'    | 2.33                     | 0.61              |
| 2:QB:115:LEU:CD2   | 2:QB:153:ARG:HD3   | 2.30                     | 0.61              |
| 33:RN:23:LEU:HD12  | 33:RN:99:LEU:HD23  | 1.82                     | 0.61              |
| 34:RO:7:TYR:HE1    | 34:RO:20:MET:HE3   | 1.65                     | 0.61              |
| 34:RO:104:ARG:CZ   | 39:RT:34:VAL:HG11  | 2.29                     | 0.61              |
| 36:RQ:2:LEU:HD23   | 36:RQ:2:LEU:H      | 1.65                     | 0.61              |
| 39:RT:49:VAL:HG13  | 39:RT:49:VAL:O     | 1.99                     | 0.61              |
| 41:RV:46:VAL:O     | 41:RV:46:VAL:HG13  | 2.01                     | 0.61              |
| 42:RW:65:LEU:O     | 42:RW:66:GLU:C     | 2.43                     | 0.61              |
| 54:R8:29:LYS:HD3   | 54:R8:44:LYS:CB    | 2.30                     | 0.61              |
| 2:XB:21:ARG:HG3    | 2:XB:38:GLY:O      | 2.01                     | 0.61              |
| 4:XD:106:TYR:HE1   | 4:XD:112:VAL:O     | 1.82                     | 0.61              |
| 4:XD:162:LEU:CD1   | 4:XD:181:MET:HB3   | 2.31                     | 0.61              |
| 6:XF:10:LEU:HD13   | 6:XF:61:LEU:CD1    | 2.30                     | 0.61              |
| 10:XJ:34:VAL:CG2   | 10:XJ:74:ILE:HG22  | 2.30                     | 0.61              |
| 11:XK:121:PRO:HD2  | 11:XK:126:ARG:HD3  | 1.82                     | 0.61              |
| 15:XO:68:ARG:O     | 15:XO:72:ARG:HB2   | 2.00                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:XX:8:A:H8       | 24:XX:8:A:O5'     | 1.83                     | 0.61              |
| 25:YA:1364:G:N7    | 47:Y1:2:SER:N     | 2.48                     | 0.61              |
| 25:YA:2529:G:O6    | 55:Y9:31:LYS:NZ   | 2.34                     | 0.61              |
| 25:YA:2864:G:OP1   | 39:YT:119:LYS:HD2 | 2.01                     | 0.61              |
| 27:YD:25:THR:HG21  | 27:YD:81:ALA:CA   | 2.31                     | 0.61              |
| 27:YD:69:ARG:C     | 27:YD:71:ASP:H    | 2.08                     | 0.61              |
| 28:YE:131:ALA:HB1  | 28:YE:135:HIS:HE1 | 1.65                     | 0.61              |
| 30:YG:77:ILE:HD13  | 30:YG:82:LEU:CD1  | 2.29                     | 0.61              |
| 36:YQ:20:ALA:HB1   | 36:YQ:99:PRO:CD   | 2.29                     | 0.61              |
| 38:YS:17:ARG:HG3   | 38:YS:18:ILE:N    | 2.14                     | 0.61              |
| 38:YS:49:VAL:HG22  | 38:YS:80:LEU:HD12 | 1.83                     | 0.61              |
| 43:YX:66:LEU:O     | 43:YX:66:LEU:HD23 | 2.01                     | 0.61              |
| 48:Y2:41:ILE:HD11  | 48:Y2:44:LEU:HG   | 1.82                     | 0.61              |
| 49:Y3:5:LYS:HB2    | 49:Y3:36:VAL:HG12 | 1.82                     | 0.61              |
| 50:Y4:64:GLY:C     | 50:Y4:66:SER:H    | 2.07                     | 0.61              |
| 54:Y8:29:LYS:HD3   | 54:Y8:44:LYS:CB   | 2.30                     | 0.61              |
| 1:QA:7:G:H5'       | 1:QA:298:A:O4'    | 2.00                     | 0.61              |
| 1:QA:222:U:H2'     | 1:QA:223:U:C6     | 2.35                     | 0.61              |
| 2:QB:80:ILE:CD1    | 2:QB:208:ILE:HG23 | 2.22                     | 0.61              |
| 2:QB:194:PRO:HG2   | 2:QB:195:ASP:H    | 1.64                     | 0.61              |
| 4:QD:90:GLY:CA     | 4:QD:204:ILE:HD11 | 2.30                     | 0.61              |
| 6:QF:98:LEU:HD12   | 6:QF:98:LEU:O     | 2.01                     | 0.61              |
| 16:QP:20:VAL:HG21  | 16:QP:32:TYR:CD2  | 2.35                     | 0.61              |
| 25:RA:1496:A:H8    | 25:RA:1577:C:O2'  | 1.83                     | 0.61              |
| 25:RA:2122:U:H2'   | 25:RA:2123:G:H8   | 1.65                     | 0.61              |
| 28:RE:69:LYS:C     | 28:RE:71:GLY:H    | 2.09                     | 0.61              |
| 29:RF:63:LYS:HE2   | 29:RF:67:GLN:HB3  | 1.83                     | 0.61              |
| 33:RN:6:PRO:HG3    | 33:RN:41:ASP:HB2  | 1.83                     | 0.61              |
| 33:RN:7:LYS:CD     | 33:RN:9:VAL:H     | 2.14                     | 0.61              |
| 52:R6:41:PRO:HD2   | 52:R6:46:HIS:N    | 2.16                     | 0.61              |
| 1:XA:1301:U:H3'    | 1:XA:1302:U:H5'   | 1.82                     | 0.61              |
| 6:XF:98:LEU:HD12   | 6:XF:98:LEU:O     | 2.01                     | 0.61              |
| 9:XI:13:ALA:HB2    | 9:XI:67:GLY:O     | 1.99                     | 0.61              |
| 10:XJ:22:LYS:HD2   | 10:XJ:22:LYS:C    | 2.25                     | 0.61              |
| 15:XO:76:GLU:C     | 15:XO:78:TYR:H    | 2.08                     | 0.61              |
| 29:YF:164:ARG:HH11 | 29:YF:164:ARG:HG2 | 1.66                     | 0.61              |
| 34:YO:78:ARG:HH21  | 39:YT:103:ARG:NH2 | 1.98                     | 0.61              |
| 37:YR:38:VAL:HB    | 37:YR:39:PRO:HD3  | 1.81                     | 0.61              |
| 37:YR:44:LEU:HD22  | 37:YR:48:VAL:HG23 | 1.82                     | 0.61              |
| 1:QA:855:G:OP2     | 1:QA:871:U:N3     | 2.33                     | 0.61              |
| 2:QB:178:ARG:NH2   | 8:QH:74:PRO:HB3   | 2.12                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:QC:70:VAL:O      | 3:QC:106:VAL:HG23 | 2.01                     | 0.61              |
| 3:QC:77:ILE:C      | 3:QC:83:ARG:HB3   | 2.26                     | 0.61              |
| 7:QG:113:GLU:CB    | 7:QG:119:ARG:HG2  | 2.30                     | 0.61              |
| 14:QN:25:VAL:HG23  | 14:QN:38:GLY:C    | 2.21                     | 0.61              |
| 15:QO:5:LYS:O      | 15:QO:8:LYS:HG2   | 2.01                     | 0.61              |
| 17:QQ:65:ILE:HD12  | 17:QQ:65:ILE:N    | 2.15                     | 0.61              |
| 17:QQ:67:LYS:HA    | 17:QQ:70:ARG:NH1  | 2.15                     | 0.61              |
| 20:QT:84:LEU:O     | 20:QT:88:VAL:HG23 | 2.01                     | 0.61              |
| 25:RA:2432:A:C8    | 47:R1:33:LYS:HE2  | 2.36                     | 0.61              |
| 27:RD:35:LYS:HG2   | 27:RD:64:ILE:CG2  | 2.31                     | 0.61              |
| 36:RQ:59:ARG:C     | 36:RQ:60:ARG:CG   | 2.74                     | 0.61              |
| 40:RU:69:CYS:HB3   | 40:RU:106:PHE:CZ  | 2.36                     | 0.61              |
| 48:R2:41:ILE:HD11  | 48:R2:44:LEU:HG   | 1.82                     | 0.61              |
| 49:R3:5:LYS:HB2    | 49:R3:36:VAL:HG12 | 1.82                     | 0.61              |
| 49:R3:59:VAL:HG12  | 49:R3:60:GLU:N    | 2.16                     | 0.61              |
| 1:XA:826:C:H2'     | 1:XA:827:U:O2     | 2.01                     | 0.61              |
| 3:XC:141:VAL:O     | 3:XC:146:ALA:HB3  | 2.01                     | 0.61              |
| 6:XF:45:LEU:HD12   | 6:XF:59:TYR:HD1   | 1.66                     | 0.61              |
| 6:XF:69:GLU:O      | 6:XF:72:VAL:HG12  | 2.01                     | 0.61              |
| 13:XM:117:VAL:HG22 | 13:XM:118:ALA:N   | 2.15                     | 0.61              |
| 25:YA:1537:C:H2'   | 25:YA:1538:G:C8   | 2.36                     | 0.61              |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:HB2 | 1.83                     | 0.61              |
| 28:YE:52:LEU:HB3   | 28:YE:54:GLN:OE1  | 2.00                     | 0.61              |
| 30:YG:44:GLY:HA2   | 30:YG:88:ILE:CG1  | 2.31                     | 0.61              |
| 34:YO:91:LEU:N     | 34:YO:91:LEU:HD22 | 2.16                     | 0.61              |
| 35:YP:27:HIS:ND1   | 35:YP:27:HIS:N    | 2.49                     | 0.61              |
| 35:YP:96:THR:HG22  | 35:YP:126:VAL:HB  | 1.82                     | 0.61              |
| 38:YS:89:ARG:O     | 38:YS:90:GLY:O    | 2.19                     | 0.61              |
| 49:Y3:59:VAL:HG12  | 49:Y3:60:GLU:N    | 2.16                     | 0.61              |
| 1:QA:939:G:H1      | 1:QA:1344:C:H42   | 1.49                     | 0.61              |
| 3:QC:3:ASN:N       | 3:QC:3:ASN:ND2    | 2.48                     | 0.61              |
| 4:QD:90:GLY:HA2    | 4:QD:204:ILE:HD11 | 1.83                     | 0.61              |
| 11:QK:41:THR:HG21  | 11:QK:71:LYS:HB2  | 1.83                     | 0.61              |
| 20:QT:34:LYS:O     | 20:QT:38:LYS:HB2  | 2.01                     | 0.61              |
| 25:RA:2563:U:H4'   | 34:RO:28:SER:HA   | 1.83                     | 0.61              |
| 28:RE:52:LEU:HB3   | 28:RE:54:GLN:OE1  | 2.00                     | 0.61              |
| 30:RG:28:VAL:O     | 30:RG:31:VAL:HG12 | 2.01                     | 0.61              |
| 33:RN:58:ASP:N     | 33:RN:60:ILE:HD11 | 2.16                     | 0.61              |
| 38:RS:49:VAL:HG22  | 38:RS:80:LEU:HD12 | 1.82                     | 0.61              |
| 41:RV:15:GLU:HG3   | 41:RV:16:PRO:HD2  | 1.83                     | 0.61              |
| 42:RW:65:LEU:HD12  | 42:RW:68:ARG:NH1  | 2.11                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:RX:14:SER:O    | 43:RX:17:ALA:N    | 2.34                     | 0.61              |
| 50:R4:64:GLY:C    | 50:R4:66:SER:H    | 2.07                     | 0.61              |
| 1:XA:243:A:H4'    | 1:XA:244:U:O5'    | 2.01                     | 0.61              |
| 3:XC:13:GLY:HA3   | 14:YN:57:ARG:CZ   | 2.31                     | 0.61              |
| 4:XD:196:LEU:HD12 | 4:XD:196:LEU:N    | 2.15                     | 0.61              |
| 5:XE:42:GLY:HA2   | 5:XE:136:MET:HE1  | 1.83                     | 0.61              |
| 8:XH:6:ILE:HB     | 8:XH:85:ARG:HH12  | 1.62                     | 0.61              |
| 17:XQ:67:LYS:HA   | 17:XQ:70:ARG:NH1  | 2.15                     | 0.61              |
| 18:XR:25:THR:HG22 | 18:XR:25:THR:O    | 2.00                     | 0.61              |
| 19:XS:16:LEU:O    | 19:XS:20:LEU:HG   | 2.01                     | 0.61              |
| 25:YA:1178:C:H2'  | 25:YA:1179:C:C6   | 2.36                     | 0.61              |
| 27:YD:2:ALA:HB3   | 27:YD:20:ASP:HB3  | 1.83                     | 0.61              |
| 33:YN:7:LYS:CD    | 33:YN:9:VAL:H     | 2.14                     | 0.61              |
| 43:YX:14:SER:O    | 43:YX:17:ALA:N    | 2.34                     | 0.61              |
| 52:Y6:7:ILE:HG13  | 52:Y6:8:LYS:N     | 2.06                     | 0.61              |
| 1:QA:1205:U:H5'   | 3:QC:190:ARG:NH2  | 2.16                     | 0.60              |
| 3:QC:47:LEU:O     | 3:QC:52:LEU:HD22  | 2.01                     | 0.60              |
| 4:QD:29:PRO:CG    | 4:QD:30:LYS:HD3   | 2.28                     | 0.60              |
| 4:QD:146:ILE:HD12 | 4:QD:146:ILE:H    | 1.66                     | 0.60              |
| 6:QF:69:GLU:O     | 6:QF:72:VAL:HG12  | 2.01                     | 0.60              |
| 13:QM:9:ILE:HD12  | 13:QM:9:ILE:O     | 2.01                     | 0.60              |
| 25:RA:608:A:OP1   | 29:RF:100:THR:OG1 | 2.12                     | 0.60              |
| 25:RA:859:G:N2    | 25:RA:917:A:OP2   | 2.25                     | 0.60              |
| 37:RR:52:ILE:O    | 37:RR:55:ALA:HB3  | 2.01                     | 0.60              |
| 42:RW:28:SER:O    | 42:RW:31:GLU:N    | 2.34                     | 0.60              |
| 3:XC:77:ILE:C     | 3:XC:83:ARG:HB3   | 2.26                     | 0.60              |
| 8:XH:23:SER:HA    | 8:XH:63:LEU:CD2   | 2.24                     | 0.60              |
| 13:XM:40:ASN:HD21 | 13:XM:42:ALA:HB3  | 1.64                     | 0.60              |
| 13:XM:96:LEU:HB3  | 13:XM:97:PRO:HD2  | 1.83                     | 0.60              |
| 17:XQ:84:LEU:C    | 17:XQ:86:GLU:H    | 2.08                     | 0.60              |
| 25:YA:404:C:O2'   | 25:YA:405:U:OP2   | 2.12                     | 0.60              |
| 27:YD:54:ARG:HH11 | 27:YD:54:ARG:CG   | 2.14                     | 0.60              |
| 29:YF:108:LYS:HZ3 | 29:YF:108:LYS:HA  | 1.64                     | 0.60              |
| 32:YI:88:ILE:HG12 | 32:YI:122:GLU:H   | 1.66                     | 0.60              |
| 38:YS:99:LYS:O    | 38:YS:102:ALA:N   | 2.34                     | 0.60              |
| 39:YT:34:VAL:HG12 | 39:YT:36:GLU:HG2  | 1.83                     | 0.60              |
| 42:YW:82:LEU:HB2  | 42:YW:98:LYS:HB2  | 1.82                     | 0.60              |
| 46:Y0:11:ARG:O    | 46:Y0:14:ARG:NH2  | 2.34                     | 0.60              |
| 50:Y4:38:LYS:C    | 50:Y4:40:HIS:N    | 2.52                     | 0.60              |
| 52:Y6:41:PRO:HD2  | 52:Y6:46:HIS:N    | 2.16                     | 0.60              |
| 2:QB:141:GLU:O    | 2:QB:145:LEU:HD23 | 2.01                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:76:ARG:HD2    | 4:QD:207:TYR:HE2   | 1.66                     | 0.60              |
| 16:QP:40:ASP:OD2   | 16:QP:42:ARG:HB2   | 2.02                     | 0.60              |
| 20:QT:101:GLY:O    | 20:QT:103:GLY:N    | 2.35                     | 0.60              |
| 25:RA:1348:G:H2'   | 25:RA:1349:A:H5''  | 1.83                     | 0.60              |
| 29:RF:175:THR:O    | 29:RF:176:LEU:CB   | 2.49                     | 0.60              |
| 31:RH:126:PRO:CD   | 31:RH:127:GLU:N    | 2.64                     | 0.60              |
| 35:RP:96:THR:HG22  | 35:RP:126:VAL:HB   | 1.83                     | 0.60              |
| 41:RV:35:LEU:O     | 41:RV:35:LEU:HD23  | 2.01                     | 0.60              |
| 3:XC:47:LEU:O      | 3:XC:52:LEU:HD22   | 2.01                     | 0.60              |
| 3:XC:88:ARG:NH1    | 3:XC:101:LEU:H     | 1.99                     | 0.60              |
| 4:XD:90:GLY:CA     | 4:XD:204:ILE:HD11  | 2.31                     | 0.60              |
| 5:XE:43:LEU:HD21   | 5:XE:132:ALA:HB1   | 1.83                     | 0.60              |
| 7:XG:79:ARG:HH11   | 7:XG:79:ARG:HG2    | 1.66                     | 0.60              |
| 9:XI:3:GLN:HB3     | 9:XI:20:ARG:HG2    | 1.82                     | 0.60              |
| 16:XP:47:ASP:C     | 16:XP:49:LEU:H     | 2.09                     | 0.60              |
| 28:YE:53:PRO:HG2   | 28:YE:54:GLN:NE2   | 2.16                     | 0.60              |
| 28:YE:63:LEU:CD1   | 28:YE:64:LYS:H     | 2.04                     | 0.60              |
| 31:YH:44:VAL:HG22  | 31:YH:44:VAL:O     | 2.01                     | 0.60              |
| 33:YN:99:LEU:O     | 33:YN:103:VAL:HG23 | 2.02                     | 0.60              |
| 35:YP:13:ASN:O     | 35:YP:15:ARG:N     | 2.34                     | 0.60              |
| 36:YQ:66:ILE:CG1   | 36:YQ:67:ARG:N     | 2.64                     | 0.60              |
| 1:QA:1347:G:C8     | 9:QI:107:ARG:HB3   | 2.35                     | 0.60              |
| 2:QB:60:ASP:O      | 2:QB:64:ARG:HG2    | 2.01                     | 0.60              |
| 4:QD:149:ALA:HB3   | 4:QD:152:SER:HB2   | 1.82                     | 0.60              |
| 8:QH:49:GLU:O      | 8:QH:51:VAL:HG13   | 2.02                     | 0.60              |
| 11:QK:78:GLN:O     | 11:QK:103:LEU:HA   | 2.01                     | 0.60              |
| 15:QO:74:ASP:OD1   | 15:QO:77:ARG:HG2   | 2.00                     | 0.60              |
| 16:QP:8:ARG:HH11   | 16:QP:8:ARG:HG2    | 1.64                     | 0.60              |
| 25:RA:2119:A:N6    | 25:RA:2170:A:N7    | 2.49                     | 0.60              |
| 27:RD:35:LYS:NZ    | 27:RD:65:ILE:HA    | 2.15                     | 0.60              |
| 27:RD:263:ARG:HH11 | 27:RD:263:ARG:CB   | 2.14                     | 0.60              |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:HG23 | 1.82                     | 0.60              |
| 30:RG:94:LEU:HD23  | 30:RG:94:LEU:H     | 1.64                     | 0.60              |
| 34:RO:91:LEU:HD22  | 34:RO:91:LEU:N     | 2.16                     | 0.60              |
| 36:RQ:66:ILE:CG1   | 36:RQ:67:ARG:N     | 2.64                     | 0.60              |
| 41:RV:66:ARG:HH12  | 41:RV:88:ARG:HH11  | 1.49                     | 0.60              |
| 1:XA:1348:U:H3     | 1:XA:1374:A:H2     | 1.46                     | 0.60              |
| 2:XB:90:MET:HE2    | 2:XB:90:MET:HA     | 1.83                     | 0.60              |
| 3:XC:70:VAL:O      | 3:XC:106:VAL:HG23  | 2.01                     | 0.60              |
| 13:XM:4:ILE:H      | 13:XM:9:ILE:HG22   | 1.62                     | 0.60              |
| 27:YD:263:ARG:HH11 | 27:YD:263:ARG:CB   | 2.15                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:YG:28:VAL:O    | 30:YG:31:VAL:HG12 | 2.01                     | 0.60              |
| 41:YV:41:GLY:H    | 41:YV:46:VAL:HG13 | 1.66                     | 0.60              |
| 44:YY:101:LYS:HE3 | 44:YY:102:CYS:SG  | 2.40                     | 0.60              |
| 1:QA:1151:A:H2'   | 1:QA:1152:A:H8    | 1.66                     | 0.60              |
| 2:QB:17:PHE:CD2   | 2:QB:44:LEU:HD11  | 2.36                     | 0.60              |
| 2:QB:221:LEU:HD13 | 2:QB:221:LEU:O    | 2.02                     | 0.60              |
| 3:QC:88:ARG:O     | 3:QC:99:VAL:HG21  | 2.01                     | 0.60              |
| 6:QF:1:MET:HA     | 6:QF:67:MET:O     | 2.02                     | 0.60              |
| 9:QI:3:GLN:HB3    | 9:QI:20:ARG:HG2   | 1.82                     | 0.60              |
| 10:QJ:32:ALA:H    | 10:QJ:78:ASN:HD21 | 1.49                     | 0.60              |
| 10:QJ:89:ASP:C    | 10:QJ:90:LEU:HD12 | 2.26                     | 0.60              |
| 14:QN:23:ARG:HD2  | 14:QN:28:GLY:O    | 2.00                     | 0.60              |
| 25:RA:519:U:H2'   | 25:RA:520:G:H8    | 1.65                     | 0.60              |
| 34:RO:104:ARG:HG2 | 34:RO:104:ARG:NH1 | 2.14                     | 0.60              |
| 43:RX:43:VAL:CG1  | 43:RX:51:VAL:HG21 | 2.31                     | 0.60              |
| 48:R2:70:GLN:O    | 48:R2:71:ASN:HB2  | 2.00                     | 0.60              |
| 2:XB:60:ASP:O     | 2:XB:64:ARG:HG2   | 2.01                     | 0.60              |
| 3:XC:130:VAL:O    | 3:XC:134:ILE:HG12 | 2.01                     | 0.60              |
| 6:XF:61:LEU:HB3   | 6:XF:63:TYR:HE2   | 1.67                     | 0.60              |
| 8:XH:49:GLU:O     | 8:XH:51:VAL:HG13  | 2.02                     | 0.60              |
| 16:XP:40:ASP:OD2  | 16:XP:42:ARG:HB2  | 2.02                     | 0.60              |
| 25:YA:27:G:N2     | 25:YA:512:G:H2'   | 2.16                     | 0.60              |
| 25:YA:297:C:H5''  | 44:YY:85:VAL:HG21 | 1.82                     | 0.60              |
| 25:YA:1799:G:OP1  | 27:YD:260:ARG:HB2 | 2.00                     | 0.60              |
| 27:YD:35:LYS:HG2  | 27:YD:64:ILE:CG2  | 2.31                     | 0.60              |
| 42:YW:36:LEU:HD11 | 42:YW:47:VAL:HG12 | 1.83                     | 0.60              |
| 1:QA:1124:G:H3'   | 1:QA:1145:C:N4    | 2.16                     | 0.60              |
| 2:QB:114:ARG:O    | 2:QB:117:GLU:HB2  | 2.01                     | 0.60              |
| 2:QB:178:ARG:HD2  | 8:QH:71:GLY:CA    | 2.31                     | 0.60              |
| 3:QC:88:ARG:NH1   | 3:QC:101:LEU:H    | 1.99                     | 0.60              |
| 4:QD:196:LEU:N    | 4:QD:196:LEU:HD12 | 2.15                     | 0.60              |
| 8:QH:86:ILE:HG22  | 8:QH:93:VAL:HG21  | 1.84                     | 0.60              |
| 16:QP:20:VAL:HG22 | 16:QP:21:VAL:N    | 2.16                     | 0.60              |
| 19:QS:12:ASP:OD1  | 19:QS:37:ARG:HD2  | 2.00                     | 0.60              |
| 30:RG:50:ALA:O    | 30:RG:53:LEU:HB3  | 2.01                     | 0.60              |
| 30:RG:61:ALA:HB2  | 30:RG:68:PRO:HD2  | 1.80                     | 0.60              |
| 30:RG:64:THR:HG23 | 30:RG:66:GLN:H    | 1.67                     | 0.60              |
| 31:RH:44:VAL:HG22 | 31:RH:44:VAL:O    | 2.01                     | 0.60              |
| 33:RN:17:ASP:O    | 33:RN:18:ALA:HB3  | 2.01                     | 0.60              |
| 35:RP:13:ASN:C    | 35:RP:15:ARG:N    | 2.54                     | 0.60              |
| 35:RP:55:ARG:HD2  | 35:RP:56:SER:O    | 2.01                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:RQ:54:MET:O     | 36:RQ:57:HIS:HB3  | 2.00                     | 0.60              |
| 40:RU:79:PHE:CD2   | 40:RU:79:PHE:C    | 2.78                     | 0.60              |
| 46:R0:68:GLU:HG2   | 46:R0:80:HIS:HB2  | 1.83                     | 0.60              |
| 2:XB:69:LEU:O      | 2:XB:162:ILE:HA   | 2.02                     | 0.60              |
| 2:XB:141:GLU:O     | 2:XB:145:LEU:HD23 | 2.01                     | 0.60              |
| 2:XB:221:LEU:HD13  | 2:XB:221:LEU:O    | 2.02                     | 0.60              |
| 3:XC:70:VAL:HG12   | 3:XC:72:LYS:N     | 2.10                     | 0.60              |
| 4:XD:146:ILE:HD12  | 4:XD:146:ILE:H    | 1.66                     | 0.60              |
| 5:XE:79:GLU:HB3    | 5:XE:92:LYS:HA    | 1.84                     | 0.60              |
| 8:XH:39:LEU:O      | 8:XH:45:ILE:HG12  | 2.01                     | 0.60              |
| 9:XI:96:LEU:HD23   | 9:XI:102:LEU:HD12 | 1.84                     | 0.60              |
| 11:XK:78:GLN:O     | 11:XK:103:LEU:HA  | 2.01                     | 0.60              |
| 13:XM:9:ILE:HD12   | 13:XM:9:ILE:O     | 2.02                     | 0.60              |
| 13:XM:37:THR:CG2   | 13:XM:39:ILE:HD11 | 2.32                     | 0.60              |
| 14:XN:44:LEU:HD12  | 14:XN:48:ALA:HB2  | 1.83                     | 0.60              |
| 20:XT:104:LEU:HD12 | 20:XT:105:SER:H   | 1.66                     | 0.60              |
| 28:YE:37:ARG:NE    | 28:YE:37:ARG:CA   | 2.64                     | 0.60              |
| 29:YF:34:TRP:CZ3   | 35:YP:8:PRO:HB3   | 2.37                     | 0.60              |
| 40:YU:69:CYS:HB3   | 40:YU:106:PHE:CZ  | 2.36                     | 0.60              |
| 40:YU:90:VAL:CG1   | 40:YU:91:ASP:H    | 2.00                     | 0.60              |
| 41:YV:35:LEU:HD23  | 41:YV:35:LEU:O    | 2.01                     | 0.60              |
| 47:Y1:3:LYS:HD3    | 47:Y1:43:TYR:CD2  | 2.35                     | 0.60              |
| 47:Y1:80:LEU:O     | 47:Y1:81:LYS:HD2  | 2.00                     | 0.60              |
| 52:Y6:13:CYS:O     | 52:Y6:21:TYR:HA   | 2.02                     | 0.60              |
| 1:QA:266:G:O2'     | 1:QA:267:C:OP2    | 2.14                     | 0.60              |
| 1:QA:501:C:H2'     | 1:QA:502:G:H8     | 1.65                     | 0.60              |
| 2:QB:90:MET:HE2    | 2:QB:90:MET:HA    | 1.83                     | 0.60              |
| 5:QE:43:LEU:HD21   | 5:QE:132:ALA:HB1  | 1.82                     | 0.60              |
| 6:QF:61:LEU:HB3    | 6:QF:63:TYR:HE2   | 1.67                     | 0.60              |
| 6:QF:89:MET:HE1    | 18:QR:76:LEU:HD22 | 1.82                     | 0.60              |
| 9:QI:28:VAL:HG13   | 9:QI:63:ILE:HG22  | 1.83                     | 0.60              |
| 16:QP:47:ASP:C     | 16:QP:49:LEU:H    | 2.09                     | 0.60              |
| 24:QX:8:A:H8       | 24:QX:8:A:O5'     | 1.83                     | 0.60              |
| 25:RA:1203:G:O6    | 25:RA:1204:A:N6   | 2.34                     | 0.60              |
| 25:RA:1332:G:N2    | 25:RA:1609:A:O2'  | 2.35                     | 0.60              |
| 25:RA:2250:G:C6    | 36:RQ:82:ARG:HD2  | 2.36                     | 0.60              |
| 25:RA:2848:G:O2'   | 25:RA:2849:U:OP2  | 2.16                     | 0.60              |
| 28:RE:4:ILE:CD1    | 28:RE:28:ALA:HB1  | 2.29                     | 0.60              |
| 33:RN:133:GLN:O    | 33:RN:134:ARG:HB3 | 1.99                     | 0.60              |
| 44:RY:44:ILE:HG13  | 44:RY:45:VAL:H    | 1.65                     | 0.60              |
| 48:R2:41:ILE:HG12  | 48:R2:44:LEU:HD12 | 1.82                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:XB:178:ARG:NE    | 8:XH:71:GLY:O      | 2.34                     | 0.60              |
| 5:XE:33:VAL:HG11   | 5:XE:109:ILE:HA    | 1.83                     | 0.60              |
| 5:XE:74:GLY:O      | 5:XE:115:VAL:HA    | 2.01                     | 0.60              |
| 10:XJ:5:ARG:O      | 10:XJ:98:ILE:HA    | 2.01                     | 0.60              |
| 13:XM:3:ARG:HA     | 13:XM:9:ILE:CG2    | 2.21                     | 0.60              |
| 17:XQ:41:LYS:HZ3   | 17:XQ:92:ARG:HH22  | 1.48                     | 0.60              |
| 19:XS:11:VAL:O     | 19:XS:12:ASP:HB2   | 2.00                     | 0.60              |
| 33:YN:16:ILE:O     | 33:YN:55:VAL:HG22  | 2.01                     | 0.60              |
| 33:YN:17:ASP:O     | 33:YN:18:ALA:HB3   | 2.01                     | 0.60              |
| 33:YN:101:HIS:CD2  | 33:YN:101:HIS:C    | 2.79                     | 0.60              |
| 37:YR:52:ILE:O     | 37:YR:55:ALA:HB3   | 2.01                     | 0.60              |
| 3:QC:141:VAL:O     | 3:QC:146:ALA:HB3   | 2.01                     | 0.60              |
| 7:QG:148:ASN:C     | 7:QG:150:ALA:H     | 2.08                     | 0.60              |
| 8:QH:58:TYR:O      | 8:QH:59:LEU:HD23   | 2.00                     | 0.60              |
| 9:QI:85:LEU:O      | 9:QI:85:LEU:HD12   | 2.02                     | 0.60              |
| 12:QL:54:LYS:CD    | 12:QL:54:LYS:N     | 2.64                     | 0.60              |
| 14:QN:15:LYS:HD2   | 14:QN:16:PHE:CZ    | 2.37                     | 0.60              |
| 20:QT:104:LEU:HD12 | 20:QT:105:SER:H    | 1.66                     | 0.60              |
| 25:RA:479:A:N3     | 25:RA:481:G:H5''   | 2.17                     | 0.60              |
| 29:RF:34:TRP:CZ3   | 35:RP:8:PRO:HB3    | 2.36                     | 0.60              |
| 29:RF:46:ARG:HH11  | 29:RF:46:ARG:CG    | 2.04                     | 0.60              |
| 32:RI:52:ARG:HB2   | 32:RI:56:LYS:HB3   | 1.83                     | 0.60              |
| 33:RN:99:LEU:O     | 33:RN:103:VAL:HG23 | 2.02                     | 0.60              |
| 43:RX:15:GLU:N     | 43:RX:15:GLU:OE1   | 2.34                     | 0.60              |
| 44:RY:19:LYS:O     | 44:RY:19:LYS:HG3   | 2.01                     | 0.60              |
| 2:XB:114:ARG:O     | 2:XB:117:GLU:HB2   | 2.01                     | 0.60              |
| 4:XD:129:ASN:HA    | 4:XD:145:GLU:HB2   | 1.82                     | 0.60              |
| 7:XG:113:GLU:CB    | 7:XG:119:ARG:HG2   | 2.29                     | 0.60              |
| 9:XI:85:LEU:HD12   | 9:XI:85:LEU:O      | 2.02                     | 0.60              |
| 12:XL:5:PRO:HA     | 12:XL:9:GLN:NE2    | 2.17                     | 0.60              |
| 25:YA:247:G:H4'    | 25:YA:386:G:C5     | 2.37                     | 0.60              |
| 25:YA:1427:A:H4'   | 25:YA:1428:C:O5'   | 2.01                     | 0.60              |
| 25:YA:2502:G:H5''  | 25:YA:2503:A:H5''  | 1.84                     | 0.60              |
| 27:YD:21:PHE:HB3   | 27:YD:24:ILE:HG13  | 1.83                     | 0.60              |
| 27:YD:147:LEU:HD13 | 27:YD:155:LEU:CD1  | 2.29                     | 0.60              |
| 27:YD:166:GLN:HE21 | 27:YD:166:GLN:CA   | 2.14                     | 0.60              |
| 28:YE:93:VAL:N     | 28:YE:95:ILE:HD12  | 2.17                     | 0.60              |
| 29:YF:175:THR:O    | 29:YF:176:LEU:CB   | 2.49                     | 0.60              |
| 30:YG:111:LEU:HB2  | 30:YG:112:PRO:HD3  | 1.82                     | 0.60              |
| 33:YN:23:LEU:HD12  | 33:YN:99:LEU:HD23  | 1.82                     | 0.60              |
| 34:YO:97:ARG:N     | 34:YO:117:LEU:HD22 | 2.15                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:60:ARG:HH11 | 45:YZ:113:ALA:HB3 | 1.66                     | 0.60              |
| 36:YQ:63:LYS:HE2  | 36:YQ:65:PHE:CE1  | 2.37                     | 0.60              |
| 38:YS:11:LYS:HB2  | 38:YS:91:PRO:HD3  | 1.84                     | 0.60              |
| 40:YU:92:ARG:NH1  | 40:YU:95:LEU:CD1  | 2.65                     | 0.60              |
| 41:YV:99:ILE:N    | 41:YV:99:ILE:CD1  | 2.65                     | 0.60              |
| 42:YW:65:LEU:O    | 42:YW:66:GLU:C    | 2.43                     | 0.60              |
| 43:YX:43:VAL:CG1  | 43:YX:51:VAL:HG21 | 2.31                     | 0.60              |
| 54:Y8:53:PRO:CD   | 54:Y8:54:GLU:H    | 2.15                     | 0.60              |
| 1:QA:1226:C:O2'   | 13:QM:111:LYS:NZ  | 2.34                     | 0.60              |
| 3:QC:130:VAL:O    | 3:QC:134:ILE:HG12 | 2.01                     | 0.60              |
| 4:QD:11:LEU:O     | 4:QD:14:ARG:N     | 2.35                     | 0.60              |
| 5:QE:131:ILE:O    | 5:QE:134:ALA:HB3  | 2.01                     | 0.60              |
| 9:QI:9:ARG:CB     | 9:QI:14:VAL:HG22  | 2.32                     | 0.60              |
| 9:QI:114:TYR:O    | 9:QI:114:TYR:HD2  | 1.85                     | 0.60              |
| 15:QO:4:THR:HB    | 15:QO:6:GLU:OE2   | 2.02                     | 0.60              |
| 17:QQ:76:LEU:HD12 | 17:QQ:77:VAL:H    | 1.66                     | 0.60              |
| 25:RA:468:G:N7    | 53:R7:39:ARG:NH2  | 2.50                     | 0.60              |
| 25:RA:1930:G:H2'  | 25:RA:1968:G:N1   | 2.16                     | 0.60              |
| 25:RA:2271:G:H2'  | 25:RA:2272:U:H6   | 1.67                     | 0.60              |
| 25:RA:2788:C:O2'  | 25:RA:2809:A:N3   | 2.32                     | 0.60              |
| 28:RE:53:PRO:HG2  | 28:RE:54:GLN:NE2  | 2.16                     | 0.60              |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CD1 | 2.37                     | 0.60              |
| 48:R2:32:LEU:HD11 | 48:R2:54:LYS:HG3  | 1.84                     | 0.60              |
| 1:XA:714:G:H2'    | 1:XA:715:A:C8     | 2.36                     | 0.60              |
| 1:XA:1053:G:H5'   | 1:XA:1054:C:H5'   | 1.84                     | 0.60              |
| 1:XA:1073:U:O2'   | 2:XB:104:ASN:OD1  | 2.13                     | 0.60              |
| 3:XC:3:ASN:N      | 3:XC:3:ASN:ND2    | 2.48                     | 0.60              |
| 4:XD:90:GLY:HA2   | 4:XD:204:ILE:HD11 | 1.83                     | 0.60              |
| 6:XF:1:MET:HA     | 6:XF:67:MET:O     | 2.02                     | 0.60              |
| 9:XI:9:ARG:CB     | 9:XI:14:VAL:HG22  | 2.31                     | 0.60              |
| 10:XJ:89:ASP:C    | 10:XJ:90:LEU:HD12 | 2.25                     | 0.60              |
| 18:XR:57:GLY:O    | 18:XR:58:LEU:C    | 2.44                     | 0.60              |
| 25:YA:558:G:P     | 33:YN:111:PRO:HD2 | 2.41                     | 0.60              |
| 25:YA:1203:G:O6   | 25:YA:1204:A:N6   | 2.35                     | 0.60              |
| 25:YA:1862:G:H2'  | 25:YA:1863:G:H8   | 1.67                     | 0.60              |
| 25:YA:2306:C:H3'  | 25:YA:2307:G:H5'' | 1.83                     | 0.60              |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HA   | 1.84                     | 0.60              |
| 27:YD:72:LYS:HE3  | 27:YD:75:ILE:HD12 | 1.82                     | 0.60              |
| 28:YE:93:VAL:N    | 28:YE:95:ILE:CD1  | 2.65                     | 0.60              |
| 4:QD:96:LEU:H     | 4:QD:96:LEU:CD2   | 2.11                     | 0.60              |
| 4:QD:114:ARG:HG3  | 4:QD:114:ARG:NH1  | 2.13                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:QJ:29:ARG:HG2    | 10:QJ:29:ARG:O     | 2.00                     | 0.60              |
| 19:QS:25:LYS:O      | 19:QS:26:GLY:O     | 2.20                     | 0.60              |
| 27:RD:2:ALA:HB3     | 27:RD:20:ASP:HB3   | 1.83                     | 0.60              |
| 27:RD:25:THR:HG21   | 27:RD:81:ALA:CA    | 2.31                     | 0.60              |
| 28:RE:37:ARG:NE     | 28:RE:37:ARG:CA    | 2.64                     | 0.60              |
| 28:RE:95:ILE:HD12   | 28:RE:95:ILE:N     | 2.14                     | 0.60              |
| 29:RF:164:ARG:HH11  | 29:RF:164:ARG:HG2  | 1.66                     | 0.60              |
| 30:RG:44:GLY:HA2    | 30:RG:88:ILE:CG1   | 2.30                     | 0.60              |
| 30:RG:128:ARG:HG3   | 30:RG:128:ARG:NH2  | 2.17                     | 0.60              |
| 30:RG:179:PRO:HG3   | 50:R4:38:LYS:HZ2   | 1.66                     | 0.60              |
| 31:RH:30:LYS:CD     | 31:RH:81:GLU:H     | 2.15                     | 0.60              |
| 31:RH:89:ILE:O      | 31:RH:91:GLY:N     | 2.35                     | 0.60              |
| 35:RP:13:ASN:O      | 35:RP:15:ARG:N     | 2.34                     | 0.60              |
| 36:RQ:97:VAL:HG21   | 36:RQ:103:MET:HE3  | 1.83                     | 0.60              |
| 37:RR:44:LEU:O      | 37:RR:48:VAL:HG23  | 2.02                     | 0.60              |
| 37:RR:44:LEU:HD22   | 37:RR:48:VAL:HG23  | 1.82                     | 0.60              |
| 38:RS:17:ARG:HG3    | 38:RS:18:ILE:N     | 2.14                     | 0.60              |
| 41:RV:18:LEU:HB3    | 41:RV:96:ILE:HG12  | 1.84                     | 0.60              |
| 2:XB:142:LEU:HD23   | 2:XB:142:LEU:C     | 2.27                     | 0.60              |
| 20:XT:74:LYS:C      | 20:XT:76:ALA:H     | 2.10                     | 0.60              |
| 25:YA:141:A:H8      | 25:YA:1408:C:H1'   | 1.67                     | 0.60              |
| 25:YA:1542:G:O6     | 25:YA:1543:A:N6    | 2.34                     | 0.60              |
| 25:YA:2394:C:OP1    | 35:YP:63:PRO:HD2   | 2.02                     | 0.60              |
| 27:YD:35:LYS:HD3    | 27:YD:63:ARG:CB    | 2.32                     | 0.60              |
| 41:YV:66:ARG:HH12   | 41:YV:88:ARG:HH11  | 1.49                     | 0.60              |
| 2:QB:4:GLU:CG       | 2:QB:5:ILE:H       | 2.00                     | 0.60              |
| 3:QC:189:ALA:HB3    | 3:QC:196:LEU:HB2   | 1.84                     | 0.60              |
| 5:QE:74:GLY:O       | 5:QE:115:VAL:HA    | 2.01                     | 0.60              |
| 12:QL:48:PRO:CD     | 12:QL:49:ASN:N     | 2.57                     | 0.60              |
| 13:QM:37:THR:CG2    | 13:QM:39:ILE:HD11  | 2.32                     | 0.60              |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:HH22  | 1.66                     | 0.60              |
| 25:RA:2576:G:O2'    | 25:RA:2579:C:OP2   | 2.16                     | 0.60              |
| 27:RD:28:GLU:O      | 27:RD:29:PRO:C     | 2.45                     | 0.60              |
| 27:RD:35:LYS:HD3    | 27:RD:63:ARG:CB    | 2.32                     | 0.60              |
| 27:RD:69:ARG:C      | 27:RD:71:ASP:H     | 2.08                     | 0.60              |
| 27:RD:165:ILE:HA    | 27:RD:175:LEU:HD23 | 1.83                     | 0.60              |
| 28:RE:26:ILE:HD13   | 28:RE:26:ILE:C     | 2.26                     | 0.60              |
| 28:RE:63:LEU:CD1    | 28:RE:64:LYS:H     | 2.04                     | 0.60              |
| 30:RG:126:ASP:OD1   | 30:RG:130:ASN:HB2  | 2.02                     | 0.60              |
| 38:RS:99:LYS:O      | 38:RS:102:ALA:N    | 2.34                     | 0.60              |
| 39:RT:34:VAL:HG12   | 39:RT:36:GLU:HG2   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:RU:76:TYR:CZ   | 40:RU:80:ILE:HG13  | 2.37                     | 0.60              |
| 52:R6:20:ASN:CG   | 52:R6:21:TYR:H     | 2.09                     | 0.60              |
| 1:XA:347:G:H1'    | 1:XA:348:G:H5''    | 1.82                     | 0.60              |
| 1:XA:1175:G:H2'   | 1:XA:1176:A:C8     | 2.37                     | 0.60              |
| 6:XF:44:GLY:HA2   | 6:XF:59:TYR:CZ     | 2.37                     | 0.60              |
| 10:XJ:32:ALA:H    | 10:XJ:78:ASN:HD21  | 1.49                     | 0.60              |
| 13:XM:97:PRO:HB2  | 13:XM:101:GLN:HE22 | 1.65                     | 0.60              |
| 16:XP:51:VAL:CG1  | 16:XP:52:ASP:N     | 2.65                     | 0.60              |
| 25:YA:67:U:H3     | 25:YA:74:A:H2      | 1.49                     | 0.60              |
| 25:YA:620:G:H4'   | 25:YA:621:A:H5'    | 1.83                     | 0.60              |
| 25:YA:1506:C:H3'  | 25:YA:1507:A:H5''  | 1.83                     | 0.60              |
| 28:YE:51:PHE:HD1  | 28:YE:52:LEU:HG    | 1.67                     | 0.60              |
| 28:YE:68:ALA:O    | 28:YE:69:LYS:HG3   | 2.02                     | 0.60              |
| 30:YG:9:ARG:HG2   | 30:YG:13:GLU:OE1   | 2.01                     | 0.60              |
| 35:YP:79:ARG:HD3  | 35:YP:110:TYR:HE1  | 1.67                     | 0.60              |
| 38:YS:59:LYS:HG2  | 38:YS:60:GLY:N     | 2.12                     | 0.60              |
| 40:YU:92:ARG:HD3  | 40:YU:94:ASN:HB3   | 1.82                     | 0.60              |
| 47:Y1:81:LYS:HA   | 47:Y1:81:LYS:HZ3   | 0.69                     | 0.60              |
| 1:QA:1342:C:H4'   | 9:QI:125:TYR:HB3   | 1.84                     | 0.59              |
| 2:QB:124:SER:HB2  | 2:QB:125:PRO:HD2   | 1.84                     | 0.59              |
| 8:QH:41:ARG:HH11  | 8:QH:41:ARG:HB3    | 1.65                     | 0.59              |
| 13:QM:96:LEU:HB3  | 13:QM:97:PRO:HD2   | 1.83                     | 0.59              |
| 20:QT:96:GLY:O    | 20:QT:97:ALA:HB3   | 2.02                     | 0.59              |
| 25:RA:1153:C:OP1  | 40:RU:76:TYR:OH    | 2.20                     | 0.59              |
| 28:RE:116:VAL:O   | 28:RE:117:MET:CB   | 2.49                     | 0.59              |
| 30:RG:180:PHE:C   | 30:RG:182:LYS:H    | 2.09                     | 0.59              |
| 35:RP:27:HIS:N    | 35:RP:27:HIS:ND1   | 2.49                     | 0.59              |
| 35:RP:88:LEU:C    | 35:RP:90:ARG:N     | 2.60                     | 0.59              |
| 37:RR:92:GLY:H    | 37:RR:94:TYR:HE2   | 1.49                     | 0.59              |
| 41:RV:35:LEU:HB2  | 41:RV:37:VAL:HG23  | 1.84                     | 0.59              |
| 44:RY:4:LYS:O     | 44:RY:5:MET:HB2    | 2.01                     | 0.59              |
| 9:XI:111:ARG:HG2  | 9:XI:112:LYS:N     | 2.16                     | 0.59              |
| 10:XJ:98:ILE:HD12 | 10:XJ:98:ILE:N     | 2.15                     | 0.59              |
| 12:XL:54:LYS:CD   | 12:XL:54:LYS:N     | 2.64                     | 0.59              |
| 19:XS:25:LYS:O    | 19:XS:26:GLY:O     | 2.20                     | 0.59              |
| 27:YD:35:LYS:CG   | 27:YD:64:ILE:N     | 2.56                     | 0.59              |
| 29:YF:63:LYS:HE2  | 29:YF:67:GLN:HB3   | 1.83                     | 0.59              |
| 30:YG:180:PHE:C   | 30:YG:182:LYS:H    | 2.09                     | 0.59              |
| 31:YH:30:LYS:CD   | 31:YH:81:GLU:H     | 2.15                     | 0.59              |
| 33:YN:1:MET:HE1   | 40:YU:95:LEU:CD2   | 2.18                     | 0.59              |
| 33:YN:18:ALA:HB3  | 33:YN:55:VAL:O     | 2.02                     | 0.59              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:YP:121:LYS:HG3   | 35:YP:122:PRO:HD2  | 1.84                     | 0.59              |
| 39:YT:107:ASP:O     | 39:YT:110:ILE:HG22 | 2.02                     | 0.59              |
| 41:YV:35:LEU:HB2    | 41:YV:37:VAL:HG23  | 1.84                     | 0.59              |
| 52:Y6:41:PRO:HG2    | 52:Y6:45:LYS:N     | 2.10                     | 0.59              |
| 54:Y8:22:VAL:CG2    | 54:Y8:53:PRO:HB2   | 2.32                     | 0.59              |
| 1:QA:15:G:H4'       | 5:QE:24:ARG:NH1    | 2.17                     | 0.59              |
| 3:QC:13:GLY:HA3     | 14:QN:57:ARG:CZ    | 2.31                     | 0.59              |
| 10:QJ:5:ARG:O       | 10:QJ:98:ILE:HA    | 2.01                     | 0.59              |
| 11:QK:34:ASP:HB3    | 11:QK:40:ILE:HD11  | 1.83                     | 0.59              |
| 25:RA:1127:A:N1     | 25:RA:2463:C:O2'   | 2.32                     | 0.59              |
| 27:RD:166:GLN:CA    | 27:RD:166:GLN:HE21 | 2.14                     | 0.59              |
| 28:RE:68:ALA:O      | 28:RE:69:LYS:HG3   | 2.02                     | 0.59              |
| 28:RE:131:ALA:HB1   | 28:RE:135:HIS:HE1  | 1.65                     | 0.59              |
| 35:RP:95:VAL:HG13   | 35:RP:100:LEU:HD21 | 1.83                     | 0.59              |
| 39:RT:6:LEU:O       | 39:RT:7:ILE:C      | 2.44                     | 0.59              |
| 39:RT:107:ASP:O     | 39:RT:110:ILE:HG22 | 2.02                     | 0.59              |
| 47:R1:91:LYS:CG     | 47:R1:92:LYS:H     | 2.15                     | 0.59              |
| 3:XC:88:ARG:O       | 3:XC:99:VAL:HG21   | 2.01                     | 0.59              |
| 7:XG:23:VAL:HG12    | 7:XG:27:ILE:CD1    | 2.32                     | 0.59              |
| 9:XI:66:ARG:HH11    | 9:XI:66:ARG:HG2    | 1.68                     | 0.59              |
| 11:XK:41:THR:HG21   | 11:XK:71:LYS:HB2   | 1.83                     | 0.59              |
| 16:XP:20:VAL:HG22   | 16:XP:21:VAL:N     | 2.16                     | 0.59              |
| 17:XQ:84:LEU:C      | 17:XQ:86:GLU:N     | 2.60                     | 0.59              |
| 20:XT:58:LYS:O      | 20:XT:62:LEU:HD12  | 2.01                     | 0.59              |
| 25:YA:242:G:H5''    | 54:Y8:3:LYS:HE3    | 1.83                     | 0.59              |
| 25:YA:607:U:H3      | 25:YA:621:A:H2     | 1.48                     | 0.59              |
| 25:YA:1490:A:O2'    | 27:YD:99:ASP:OD2   | 2.19                     | 0.59              |
| 27:YD:172:TYR:CD1   | 27:YD:186:HIS:HA   | 2.37                     | 0.59              |
| 28:YE:116:VAL:O     | 28:YE:117:MET:CB   | 2.49                     | 0.59              |
| 29:YF:123:LEU:HD12  | 29:YF:124:LEU:N    | 2.17                     | 0.59              |
| 30:YG:50:ALA:O      | 30:YG:53:LEU:HB3   | 2.01                     | 0.59              |
| 35:YP:55:ARG:HD2    | 35:YP:56:SER:O     | 2.01                     | 0.59              |
| 35:YP:88:LEU:C      | 35:YP:90:ARG:N     | 2.60                     | 0.59              |
| 52:Y6:25:LYS:HD2    | 54:Y8:34:TRP:CZ2   | 2.36                     | 0.59              |
| 2:QB:188:ALA:HB3    | 2:QB:200:ILE:HG23  | 1.84                     | 0.59              |
| 6:QF:44:GLY:HA2     | 6:QF:59:TYR:CZ     | 2.37                     | 0.59              |
| 7:QG:66:VAL:O       | 7:QG:70:LYS:HG3    | 2.02                     | 0.59              |
| 17:QQ:84:LEU:C      | 17:QQ:86:GLU:H     | 2.08                     | 0.59              |
| 25:RA:1444(A):A:H4' | 25:RA:1460:A:O2'   | 2.02                     | 0.59              |
| 26:RB:42:C:C6       | 30:RG:69:ALA:HB2   | 2.37                     | 0.59              |
| 27:RD:172:TYR:CD1   | 27:RD:186:HIS:HA   | 2.37                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:61:ARG:HB2  | 28:RE:62:PRO:CD    | 2.33                     | 0.59              |
| 28:RE:69:LYS:O    | 28:RE:71:GLY:N     | 2.27                     | 0.59              |
| 29:RF:155:LEU:CD1 | 29:RF:174:VAL:HG13 | 2.32                     | 0.59              |
| 33:RN:16:ILE:O    | 33:RN:55:VAL:HG22  | 2.01                     | 0.59              |
| 36:RQ:63:LYS:HE2  | 36:RQ:65:PHE:CE1   | 2.37                     | 0.59              |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:H     | 1.67                     | 0.59              |
| 38:RS:11:LYS:HB2  | 38:RS:91:PRO:HD3   | 1.84                     | 0.59              |
| 40:RU:58:ARG:HA   | 40:RU:61:TRP:CE3   | 2.37                     | 0.59              |
| 45:RZ:94:GLU:HB2  | 45:RZ:130:PRO:HD2  | 1.84                     | 0.59              |
| 54:R8:22:VAL:CG2  | 54:R8:53:PRO:HB2   | 2.32                     | 0.59              |
| 2:XB:188:ALA:HB3  | 2:XB:200:ILE:HG23  | 1.83                     | 0.59              |
| 3:XC:107:GLN:CD   | 3:XC:107:GLN:N     | 2.61                     | 0.59              |
| 16:XP:43:LYS:HA   | 16:XP:48:TRP:HB2   | 1.83                     | 0.59              |
| 20:XT:47:GLY:C    | 20:XT:49:ALA:H     | 2.08                     | 0.59              |
| 25:YA:2747:G:OP1  | 31:YH:138:LYS:NZ   | 2.35                     | 0.59              |
| 39:YT:57:PHE:CD2  | 39:YT:58:ASN:N     | 2.66                     | 0.59              |
| 39:YT:102:ILE:HB  | 39:YT:110:ILE:HD13 | 1.84                     | 0.59              |
| 40:YU:92:ARG:HH11 | 40:YU:95:LEU:HD12  | 1.67                     | 0.59              |
| 44:YY:4:LYS:O     | 44:YY:5:MET:HB2    | 2.01                     | 0.59              |
| 44:YY:96:ILE:CD1  | 44:YY:98:VAL:HG12  | 2.32                     | 0.59              |
| 45:YZ:58:VAL:O    | 45:YZ:60:GLU:N     | 2.34                     | 0.59              |
| 52:Y6:20:ASN:CG   | 52:Y6:21:TYR:H     | 2.09                     | 0.59              |
| 54:Y8:56:GLU:O    | 54:Y8:59:LYS:N     | 2.36                     | 0.59              |
| 1:QA:372:C:H42    | 1:QA:389:A:H62     | 1.49                     | 0.59              |
| 3:QC:60:ALA:O     | 3:QC:61:ALA:CB     | 2.50                     | 0.59              |
| 5:QE:33:VAL:HG11  | 5:QE:109:ILE:HA    | 1.83                     | 0.59              |
| 5:QE:72:GLN:O     | 5:QE:73:ASN:HB3    | 2.02                     | 0.59              |
| 7:QG:23:VAL:HG12  | 7:QG:27:ILE:CD1    | 2.32                     | 0.59              |
| 8:QH:86:ILE:HG13  | 8:QH:133:LEU:HD22  | 1.84                     | 0.59              |
| 14:QN:44:LEU:HD12 | 14:QN:48:ALA:HB2   | 1.84                     | 0.59              |
| 19:QS:16:LEU:O    | 19:QS:20:LEU:HG    | 2.01                     | 0.59              |
| 27:RD:25:THR:HG21 | 27:RD:81:ALA:HA    | 1.84                     | 0.59              |
| 30:RG:13:GLU:O    | 30:RG:14:GLU:CB    | 2.44                     | 0.59              |
| 31:RH:4:ILE:N     | 31:RH:4:ILE:HD13   | 2.18                     | 0.59              |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:HD2  | 1.84                     | 0.59              |
| 35:RP:106:LEU:O   | 35:RP:107:LYS:CB   | 2.46                     | 0.59              |
| 39:RT:102:ILE:HB  | 39:RT:110:ILE:HD13 | 1.84                     | 0.59              |
| 52:R6:13:CYS:O    | 52:R6:21:TYR:HA    | 2.01                     | 0.59              |
| 54:R8:22:VAL:HG21 | 54:R8:53:PRO:HB2   | 1.82                     | 0.59              |
| 5:XE:72:GLN:O     | 5:XE:73:ASN:HB3    | 2.03                     | 0.59              |
| 8:XH:41:ARG:HH11  | 8:XH:41:ARG:HB3    | 1.66                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:XR:31:LEU:HD23  | 18:XR:31:LEU:H    | 1.67                     | 0.59              |
| 25:YA:819:A:OP2    | 25:YA:1187:G:N2   | 2.29                     | 0.59              |
| 31:YH:4:ILE:N      | 31:YH:4:ILE:HD13  | 2.17                     | 0.59              |
| 31:YH:55:PRO:HG2   | 31:YH:61:HIS:CE1  | 2.37                     | 0.59              |
| 33:YN:42:TRP:O     | 40:YU:64:ARG:NH2  | 2.35                     | 0.59              |
| 40:YU:58:ARG:HA    | 40:YU:61:TRP:CE3  | 2.37                     | 0.59              |
| 40:YU:76:TYR:CZ    | 40:YU:80:ILE:HG13 | 2.37                     | 0.59              |
| 44:YY:95:LYS:HD3   | 44:YY:95:LYS:H    | 1.67                     | 0.59              |
| 52:Y6:27:LYS:HB2   | 52:Y6:27:LYS:HZ3  | 1.67                     | 0.59              |
| 1:QA:971:G:N2      | 1:QA:1363:A:OP2   | 2.25                     | 0.59              |
| 2:QB:69:LEU:O      | 2:QB:162:ILE:HA   | 2.02                     | 0.59              |
| 2:QB:115:LEU:HD23  | 2:QB:153:ARG:HD3  | 1.84                     | 0.59              |
| 3:QC:149:ALA:O     | 3:QC:169:ALA:HA   | 2.02                     | 0.59              |
| 7:QG:79:ARG:HH11   | 7:QG:79:ARG:HG2   | 1.66                     | 0.59              |
| 9:QI:111:ARG:HG2   | 9:QI:112:LYS:N    | 2.16                     | 0.59              |
| 10:QJ:31:GLY:HA3   | 10:QJ:78:ASN:ND2  | 2.18                     | 0.59              |
| 11:QK:51:LYS:CA    | 11:QK:55:LYS:HD3  | 2.21                     | 0.59              |
| 12:QL:46:LYS:HG2   | 12:QL:47:LYS:H    | 1.67                     | 0.59              |
| 13:QM:45:VAL:HG22  | 13:QM:45:VAL:O    | 2.02                     | 0.59              |
| 20:QT:58:LYS:O     | 20:QT:62:LEU:HD12 | 2.02                     | 0.59              |
| 20:QT:104:LEU:HD12 | 20:QT:105:SER:N   | 2.18                     | 0.59              |
| 25:RA:1899:G:H21   | 25:RA:1902:C:N4   | 2.00                     | 0.59              |
| 27:RD:137:PRO:HB2  | 27:RD:140:THR:CG2 | 2.33                     | 0.59              |
| 33:RN:78:TYR:N     | 33:RN:78:TYR:CD1  | 2.70                     | 0.59              |
| 35:RP:79:ARG:HD3   | 35:RP:110:TYR:HE1 | 1.67                     | 0.59              |
| 38:RS:89:ARG:O     | 38:RS:90:GLY:O    | 2.19                     | 0.59              |
| 42:RW:36:LEU:HD11  | 42:RW:47:VAL:HG12 | 1.83                     | 0.59              |
| 47:R1:87:PRO:O     | 47:R1:91:LYS:N    | 2.32                     | 0.59              |
| 51:R5:52:TYR:O     | 51:R5:53:ALA:HB3  | 2.01                     | 0.59              |
| 2:XB:124:SER:HB2   | 2:XB:125:PRO:HD2  | 1.85                     | 0.59              |
| 3:XC:60:ALA:O      | 3:XC:61:ALA:CB    | 2.50                     | 0.59              |
| 4:XD:173:TRP:O     | 4:XD:186:LEU:HB2  | 2.02                     | 0.59              |
| 10:XJ:31:GLY:HA3   | 10:XJ:78:ASN:ND2  | 2.17                     | 0.59              |
| 15:XO:5:LYS:O      | 15:XO:8:LYS:HG2   | 2.02                     | 0.59              |
| 17:XQ:76:LEU:HD12  | 17:XQ:77:VAL:H    | 1.67                     | 0.59              |
| 19:XS:40:ILE:HD11  | 19:XS:62:ILE:HG21 | 1.85                     | 0.59              |
| 25:YA:482:A:O2'    | 44:YY:47:LYS:NZ   | 2.33                     | 0.59              |
| 28:YE:26:ILE:HD13  | 28:YE:26:ILE:C    | 2.27                     | 0.59              |
| 29:YF:11:VAL:HG11  | 29:YF:18:ARG:HE   | 1.67                     | 0.59              |
| 31:YH:86:GLU:O     | 31:YH:131:VAL:O   | 2.20                     | 0.59              |
| 31:YH:159:GLU:O    | 31:YH:160:LYS:HG2 | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:YR:72:ASP:O     | 37:YR:76:VAL:HB    | 2.03                     | 0.59              |
| 3:QC:36:ASP:HB3    | 3:QC:40:ARG:HH12   | 1.68                     | 0.59              |
| 6:QF:26:ILE:O      | 6:QF:30:LEU:HG     | 2.02                     | 0.59              |
| 16:QP:43:LYS:HA    | 16:QP:48:TRP:HB2   | 1.84                     | 0.59              |
| 20:QT:74:LYS:C     | 20:QT:76:ALA:H     | 2.10                     | 0.59              |
| 25:RA:864:G:H1'    | 25:RA:914:C:H42    | 1.68                     | 0.59              |
| 25:RA:1342:A:OP1   | 43:RX:36:LYS:NZ    | 2.34                     | 0.59              |
| 25:RA:1364:G:N7    | 47:R1:2:SER:N      | 2.51                     | 0.59              |
| 28:RE:174:ASP:CG   | 28:RE:175:VAL:N    | 2.58                     | 0.59              |
| 31:RH:82:GLY:O     | 31:RH:135:GLY:O    | 2.20                     | 0.59              |
| 33:RN:9:VAL:HG21   | 33:RN:48:MET:HB3   | 1.85                     | 0.59              |
| 35:RP:37:GLY:HA2   | 35:RP:41:ARG:HE    | 1.68                     | 0.59              |
| 42:RW:66:GLU:O     | 42:RW:68:ARG:N     | 2.33                     | 0.59              |
| 51:R5:40:LYS:NZ    | 51:R5:46:CYS:HB3   | 2.18                     | 0.59              |
| 53:R7:18:PHE:C     | 53:R7:18:PHE:CD2   | 2.81                     | 0.59              |
| 4:XD:22:LYS:O      | 4:XD:113:SER:HB3   | 2.03                     | 0.59              |
| 7:XG:85:TYR:HE1    | 7:XG:154:TYR:CE1   | 2.21                     | 0.59              |
| 8:XH:86:ILE:HG22   | 8:XH:93:VAL:HG21   | 1.84                     | 0.59              |
| 12:XL:46:LYS:HG2   | 12:XL:47:LYS:H     | 1.67                     | 0.59              |
| 17:XQ:92:ARG:HH11  | 17:XQ:92:ARG:HG3   | 1.68                     | 0.59              |
| 20:XT:96:GLY:O     | 20:XT:97:ALA:HB3   | 2.02                     | 0.59              |
| 20:XT:104:LEU:HD12 | 20:XT:105:SER:N    | 2.18                     | 0.59              |
| 22:XV:1:C:O2'      | 46:Y0:6:GLY:O      | 2.19                     | 0.59              |
| 25:YA:468:G:N7     | 53:Y7:39:ARG:NH2   | 2.49                     | 0.59              |
| 27:YD:174:ILE:HD12 | 27:YD:174:ILE:N    | 2.16                     | 0.59              |
| 33:YN:6:PRO:HG3    | 33:YN:41:ASP:HB2   | 1.83                     | 0.59              |
| 33:YN:78:TYR:N     | 33:YN:78:TYR:CD1   | 2.70                     | 0.59              |
| 35:YP:95:VAL:HG13  | 35:YP:100:LEU:HD21 | 1.84                     | 0.59              |
| 35:YP:127:ALA:O    | 35:YP:147:LEU:HD23 | 2.02                     | 0.59              |
| 36:YQ:97:VAL:HG21  | 36:YQ:103:MET:HE3  | 1.83                     | 0.59              |
| 39:YT:6:LEU:O      | 39:YT:7:ILE:C      | 2.45                     | 0.59              |
| 49:Y3:29:ARG:HH11  | 49:Y3:29:ARG:CB    | 2.13                     | 0.59              |
| 52:Y6:44:ARG:O     | 52:Y6:45:LYS:HB2   | 2.00                     | 0.59              |
| 1:QA:737:A:H2'     | 1:QA:738:C:C6      | 2.38                     | 0.59              |
| 2:QB:19:HIS:NE2    | 2:QB:206:ASP:HB2   | 2.18                     | 0.59              |
| 4:QD:173:TRP:O     | 4:QD:186:LEU:HB2   | 2.02                     | 0.59              |
| 5:QE:68:GLU:O      | 5:QE:68:GLU:HG3    | 2.03                     | 0.59              |
| 5:QE:79:GLU:HB3    | 5:QE:92:LYS:HA     | 1.84                     | 0.59              |
| 9:QI:9:ARG:HB3     | 9:QI:14:VAL:HG13   | 1.85                     | 0.59              |
| 10:QJ:13:HIS:HB3   | 10:QJ:68:HIS:CE1   | 2.37                     | 0.59              |
| 19:QS:5:LEU:HD21   | 50:R4:67:TYR:CE2   | 2.38                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1857:G:O2'   | 25:RA:1885:A:N6    | 2.35                     | 0.59              |
| 27:RD:54:ARG:HH11  | 27:RD:54:ARG:CG    | 2.14                     | 0.59              |
| 28:RE:36:ARG:H     | 28:RE:37:ARG:HH21  | 1.49                     | 0.59              |
| 28:RE:116:VAL:CG2  | 28:RE:122:PHE:CD2  | 2.86                     | 0.59              |
| 40:RU:52:ARG:HG2   | 40:RU:52:ARG:NH1   | 2.17                     | 0.59              |
| 47:R1:53:VAL:O     | 47:R1:54:ALA:C     | 2.45                     | 0.59              |
| 1:XA:1186:G:O3'    | 9:XI:113:LYS:NZ    | 2.34                     | 0.59              |
| 1:XA:1219:U:OP1    | 14:XN:19:ARG:NH2   | 2.34                     | 0.59              |
| 6:XF:26:ILE:O      | 6:XF:30:LEU:HG     | 2.02                     | 0.59              |
| 7:XG:66:VAL:O      | 7:XG:70:LYS:HG3    | 2.02                     | 0.59              |
| 8:XH:12:ARG:HH12   | 8:XH:27:PRO:HD2    | 1.67                     | 0.59              |
| 11:XK:69:ALA:HB1   | 11:XK:103:LEU:HD21 | 1.85                     | 0.59              |
| 14:XN:15:LYS:HD2   | 14:XN:16:PHE:CZ    | 2.37                     | 0.59              |
| 25:YA:530:G:O2'    | 25:YA:532:A:N7     | 2.36                     | 0.59              |
| 25:YA:900:A:H3'    | 25:YA:901:A:H8     | 1.67                     | 0.59              |
| 25:YA:1820:U:C2    | 27:YD:202:LYS:HB3  | 2.37                     | 0.59              |
| 25:YA:2335:A:O2'   | 25:YA:2336:A:H2'   | 2.02                     | 0.59              |
| 25:YA:2537:U:H2'   | 25:YA:2538:C:C6    | 2.37                     | 0.59              |
| 30:YG:16:ARG:NH2   | 30:YG:31:VAL:HG11  | 2.17                     | 0.59              |
| 33:YN:58:ASP:N     | 33:YN:60:ILE:HD11  | 2.16                     | 0.59              |
| 35:YP:39:LYS:CA    | 35:YP:45:LEU:CD1   | 2.80                     | 0.59              |
| 39:YT:66:VAL:HG12  | 39:YT:67:SER:H     | 1.66                     | 0.59              |
| 47:Y1:53:VAL:O     | 47:Y1:54:ALA:C     | 2.45                     | 0.59              |
| 1:QA:181:G:O2'     | 1:QA:182:U:O5'     | 2.21                     | 0.59              |
| 1:QA:581:G:N2      | 1:QA:760:G:N7      | 2.51                     | 0.59              |
| 1:QA:963:G:N3      | 10:QJ:55:LYS:NZ    | 2.51                     | 0.59              |
| 3:QC:107:GLN:CD    | 3:QC:107:GLN:N     | 2.61                     | 0.59              |
| 3:QC:127:ARG:HH11  | 3:QC:127:ARG:CG    | 2.15                     | 0.59              |
| 5:QE:78:HIS:CG     | 8:QH:104:ARG:HG2   | 2.38                     | 0.59              |
| 8:QH:41:ARG:HH11   | 8:QH:41:ARG:CG     | 2.16                     | 0.59              |
| 9:QI:40:LEU:HD11   | 9:QI:70:LYS:HG2    | 1.84                     | 0.59              |
| 9:QI:96:LEU:HD23   | 9:QI:102:LEU:HD12  | 1.84                     | 0.59              |
| 14:QN:24:CYS:SG    | 14:QN:40:CYS:N     | 2.76                     | 0.59              |
| 25:RA:898:C:H2'    | 25:RA:899:A:H5'    | 1.85                     | 0.59              |
| 29:RF:123:LEU:HD12 | 29:RF:124:LEU:N    | 2.17                     | 0.59              |
| 33:RN:18:ALA:HB3   | 33:RN:55:VAL:O     | 2.03                     | 0.59              |
| 35:RP:71:VAL:HG13  | 35:RP:72:PRO:HD3   | 1.85                     | 0.59              |
| 42:RW:20:VAL:C     | 42:RW:22:ASP:N     | 2.60                     | 0.59              |
| 44:RY:51:VAL:CG1   | 44:RY:52:SER:H     | 2.11                     | 0.59              |
| 3:XC:127:ARG:HH11  | 3:XC:127:ARG:CG    | 2.15                     | 0.59              |
| 5:XE:42:GLY:CA     | 5:XE:66:MET:HG2    | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:XE:148:VAL:HG21  | 8:XH:107:LEU:HD13  | 1.85                     | 0.59              |
| 12:XL:70:ILE:HD13  | 12:XL:77:LEU:HD12  | 1.83                     | 0.59              |
| 20:XT:84:LEU:O     | 20:XT:88:VAL:HG23  | 2.01                     | 0.59              |
| 20:XT:101:GLY:O    | 20:XT:103:GLY:N    | 2.35                     | 0.59              |
| 25:YA:2335:A:O2'   | 25:YA:2336:A:O5'   | 2.18                     | 0.59              |
| 27:YD:27:THR:CG2   | 27:YD:83:GLU:HB3   | 2.33                     | 0.59              |
| 30:YG:35:GLU:CD    | 30:YG:35:GLU:C     | 2.71                     | 0.59              |
| 31:YH:82:GLY:O     | 31:YH:135:GLY:O    | 2.20                     | 0.59              |
| 36:YQ:81:VAL:HG23  | 36:YQ:82:ARG:H     | 1.67                     | 0.59              |
| 37:YR:92:GLY:H     | 37:YR:94:TYR:HE2   | 1.49                     | 0.59              |
| 38:YS:88:ASP:O     | 38:YS:89:ARG:CB    | 2.49                     | 0.59              |
| 41:YV:15:GLU:HG3   | 41:YV:16:PRO:HD2   | 1.83                     | 0.59              |
| 50:Y4:22:ILE:HG22  | 50:Y4:23:GLU:N     | 2.18                     | 0.59              |
| 50:Y4:48:ARG:NH1   | 50:Y4:52:THR:H     | 2.01                     | 0.59              |
| 53:Y7:18:PHE:CD2   | 53:Y7:18:PHE:C     | 2.81                     | 0.59              |
| 1:QA:1459:C:OP1    | 20:QT:27:LYS:NZ    | 2.35                     | 0.59              |
| 2:QB:142:LEU:C     | 2:QB:142:LEU:HD23  | 2.27                     | 0.59              |
| 6:QF:45:LEU:HD12   | 6:QF:59:TYR:HD1    | 1.66                     | 0.59              |
| 9:QI:66:ARG:HH11   | 9:QI:66:ARG:HG2    | 1.68                     | 0.59              |
| 12:QL:5:PRO:HA     | 12:QL:9:GLN:NE2    | 2.17                     | 0.59              |
| 12:QL:54:LYS:N     | 12:QL:54:LYS:HD2   | 2.18                     | 0.59              |
| 12:QL:70:ILE:HD13  | 12:QL:77:LEU:HD12  | 1.83                     | 0.59              |
| 27:RD:71:ASP:HB3   | 27:RD:103:ARG:HH22 | 1.68                     | 0.59              |
| 28:RE:93:VAL:N     | 28:RE:95:ILE:CD1   | 2.65                     | 0.59              |
| 31:RH:127:GLU:HG2  | 31:RH:128:PRO:CG   | 2.33                     | 0.59              |
| 39:RT:36:GLU:HG3   | 39:RT:41:ARG:HD3   | 1.85                     | 0.59              |
| 45:RZ:110:GLY:HA2  | 45:RZ:111:VAL:C    | 2.27                     | 0.59              |
| 1:XA:1151:A:H2'    | 1:XA:1152:A:H8     | 1.68                     | 0.59              |
| 4:XD:11:LEU:HD22   | 4:XD:66:ARG:CD     | 2.19                     | 0.59              |
| 11:XK:30:VAL:HG21  | 11:XK:65:ALA:HA    | 1.85                     | 0.59              |
| 25:YA:330:A:HO2'   | 25:YA:331:A:H8     | 1.51                     | 0.59              |
| 25:YA:996:A:H4'    | 40:YU:92:ARG:HE    | 1.67                     | 0.59              |
| 25:YA:1094:U:O2'   | 25:YA:1096:A:OP1   | 2.16                     | 0.59              |
| 27:YD:137:PRO:HB2  | 27:YD:140:THR:CG2  | 2.33                     | 0.59              |
| 27:YD:177:LEU:HD11 | 27:YD:183:ARG:HB2  | 1.85                     | 0.59              |
| 30:YG:126:ASP:OD1  | 30:YG:130:ASN:HB2  | 2.02                     | 0.59              |
| 31:YH:124:GLU:HB3  | 31:YH:132:ARG:HG3  | 1.85                     | 0.59              |
| 31:YH:126:PRO:CD   | 31:YH:127:GLU:N    | 2.64                     | 0.59              |
| 39:YT:102:ILE:HB   | 39:YT:110:ILE:HD11 | 1.84                     | 0.59              |
| 41:YV:18:LEU:HB3   | 41:YV:96:ILE:HG12  | 1.84                     | 0.59              |
| 42:YW:20:VAL:C     | 42:YW:22:ASP:H     | 2.10                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:YX:49:VAL:CG1   | 43:YX:83:VAL:HG13  | 2.33                     | 0.59              |
| 48:Y2:64:LEU:CD2   | 48:Y2:68:ARG:HD2   | 2.33                     | 0.59              |
| 50:Y4:15:ILE:HG22  | 50:Y4:19:GLY:O     | 2.03                     | 0.59              |
| 1:QA:34:C:H2'      | 1:QA:35:G:C8       | 2.37                     | 0.59              |
| 2:QB:47:THR:HG22   | 2:QB:51:LEU:HG     | 1.85                     | 0.59              |
| 2:QB:80:ILE:HD11   | 2:QB:208:ILE:CG2   | 2.23                     | 0.59              |
| 5:QE:42:GLY:CA     | 5:QE:66:MET:HG2    | 2.32                     | 0.59              |
| 8:QH:12:ARG:HH12   | 8:QH:27:PRO:HD2    | 1.67                     | 0.59              |
| 17:QQ:92:ARG:HG3   | 17:QQ:92:ARG:HH11  | 1.67                     | 0.59              |
| 22:QV:53:G:H4'     | 22:QV:54:U:OP1     | 2.03                     | 0.59              |
| 25:RA:242:G:C8     | 54:R8:5:LYS:HG2    | 2.37                     | 0.59              |
| 26:RB:31:C:H42     | 26:RB:51:G:H1      | 1.51                     | 0.59              |
| 27:RD:44:ASN:N     | 27:RD:44:ASN:ND2   | 2.42                     | 0.59              |
| 29:RF:89:VAL:HG12  | 29:RF:90:PHE:N     | 2.18                     | 0.59              |
| 31:RH:55:PRO:HG2   | 31:RH:61:HIS:CE1   | 2.37                     | 0.59              |
| 33:RN:13:TRP:O     | 33:RN:135:PRO:HD2  | 2.03                     | 0.59              |
| 35:RP:138:LEU:O    | 35:RP:140:ALA:N    | 2.33                     | 0.59              |
| 36:RQ:63:LYS:HD2   | 45:RZ:175:VAL:HG21 | 1.83                     | 0.59              |
| 43:RX:49:VAL:CG1   | 43:RX:83:VAL:HG13  | 2.33                     | 0.59              |
| 48:R2:64:LEU:CD2   | 48:R2:68:ARG:HD2   | 2.33                     | 0.59              |
| 53:R7:31:LEU:O     | 53:R7:32:LYS:C     | 2.43                     | 0.59              |
| 1:XA:437:U:H2'     | 1:XA:438:G:O4'     | 2.03                     | 0.59              |
| 1:XA:1002:G:H1     | 1:XA:1038:C:H42    | 1.50                     | 0.59              |
| 4:XD:114:ARG:HG3   | 4:XD:114:ARG:NH1   | 2.13                     | 0.59              |
| 9:XI:9:ARG:HB3     | 9:XI:14:VAL:HG13   | 1.85                     | 0.59              |
| 19:XS:64:GLU:CD    | 50:Y4:55:ARG:HH22  | 2.10                     | 0.59              |
| 25:YA:1814:G:H4'   | 27:YD:51:VAL:HG21  | 1.85                     | 0.59              |
| 27:YD:27:THR:CG2   | 27:YD:28:GLU:N     | 2.66                     | 0.59              |
| 31:YH:4:ILE:HG13   | 31:YH:6:ARG:CD     | 2.33                     | 0.59              |
| 35:YP:138:LEU:O    | 35:YP:140:ALA:N    | 2.33                     | 0.59              |
| 41:YV:49:THR:CB    | 41:YV:50:PRO:HD2   | 2.25                     | 0.59              |
| 50:Y4:3:GLU:HG3    | 50:Y4:4:GLY:N      | 2.18                     | 0.59              |
| 51:Y5:40:LYS:NZ    | 51:Y5:46:CYS:HB3   | 2.18                     | 0.59              |
| 2:QB:187:LEU:CD1   | 2:QB:205:ASP:HA    | 2.33                     | 0.58              |
| 9:QI:17:VAL:HG13   | 9:QI:81:ILE:HD13   | 1.85                     | 0.58              |
| 9:QI:128:ARG:HD3   | 22:QV:32:C:OP2     | 2.01                     | 0.58              |
| 13:QM:84:ILE:HG23  | 13:QM:85:GLY:N     | 2.17                     | 0.58              |
| 16:QP:53:VAL:HG23  | 16:QP:54:GLU:N     | 2.18                     | 0.58              |
| 18:QR:31:LEU:HD23  | 18:QR:31:LEU:H     | 1.67                     | 0.58              |
| 25:RA:270(T):G:OP1 | 47:R1:97:LEU:HD13  | 2.02                     | 0.58              |
| 25:RA:2839:G:H5'   | 37:RR:46:GLY:HA2   | 1.84                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:92:ILE:HD12  | 27:RD:104:TYR:CD2  | 2.38                     | 0.58              |
| 28:RE:72:VAL:O     | 28:RE:73:GLU:O     | 2.21                     | 0.58              |
| 31:RH:92:ILE:HG22  | 31:RH:93:GLY:N     | 2.18                     | 0.58              |
| 32:RI:3:VAL:HG12   | 32:RI:38:LEU:HA    | 1.85                     | 0.58              |
| 35:RP:127:ALA:O    | 35:RP:147:LEU:HD23 | 2.02                     | 0.58              |
| 37:RR:72:ASP:O     | 37:RR:76:VAL:HB    | 2.03                     | 0.58              |
| 39:RT:66:VAL:HG12  | 39:RT:67:SER:H     | 1.67                     | 0.58              |
| 42:RW:20:VAL:C     | 42:RW:22:ASP:H     | 2.10                     | 0.58              |
| 50:R4:65:ASP:O     | 50:R4:66:SER:CB    | 2.51                     | 0.58              |
| 3:XC:149:ALA:O     | 3:XC:169:ALA:HA    | 2.02                     | 0.58              |
| 5:XE:153:LYS:HB2   | 5:XE:153:LYS:NZ    | 2.18                     | 0.58              |
| 8:XH:41:ARG:HH11   | 8:XH:41:ARG:CG     | 2.16                     | 0.58              |
| 9:XI:13:ALA:HB2    | 9:XI:67:GLY:C      | 2.28                     | 0.58              |
| 13:XM:121:LYS:NZ   | 23:XY:40:G:O2'     | 2.36                     | 0.58              |
| 25:YA:1678:G:N2    | 25:YA:1989:G:H22   | 2.02                     | 0.58              |
| 28:YE:36:ARG:H     | 28:YE:37:ARG:HH21  | 1.50                     | 0.58              |
| 29:YF:63:LYS:HE2   | 29:YF:67:GLN:CB    | 2.32                     | 0.58              |
| 29:YF:174:VAL:HG13 | 29:YF:174:VAL:O    | 2.03                     | 0.58              |
| 31:YH:89:ILE:O     | 31:YH:91:GLY:N     | 2.35                     | 0.58              |
| 32:YI:40:THR:O     | 32:YI:44:LEU:HB2   | 2.02                     | 0.58              |
| 37:YR:44:LEU:O     | 37:YR:48:VAL:HG23  | 2.02                     | 0.58              |
| 48:Y2:32:LEU:HD11  | 48:Y2:54:LYS:HG3   | 1.84                     | 0.58              |
| 51:Y5:52:TYR:O     | 51:Y5:53:ALA:HB3   | 2.02                     | 0.58              |
| 1:QA:1014:A:H4'    | 19:QS:14:HIS:NE2   | 2.17                     | 0.58              |
| 5:QE:102:ALA:HB2   | 5:QE:120:THR:OG1   | 2.03                     | 0.58              |
| 25:RA:270(U):C:H2' | 25:RA:270(V):G:H8  | 1.68                     | 0.58              |
| 25:RA:2224:G:OP1   | 27:RD:268:ARG:HD3  | 2.02                     | 0.58              |
| 25:RA:2405:G:O2'   | 25:RA:2411:A:N6    | 2.36                     | 0.58              |
| 25:RA:2758:A:C4    | 31:RH:67:LEU:HD21  | 2.38                     | 0.58              |
| 28:RE:93:VAL:N     | 28:RE:95:ILE:HD12  | 2.17                     | 0.58              |
| 32:RI:78:THR:HG22  | 32:RI:141:LYS:HD2  | 1.85                     | 0.58              |
| 33:RN:114:ARG:O    | 33:RN:115:ARG:HB3  | 2.03                     | 0.58              |
| 35:RP:121:LYS:HG3  | 35:RP:122:PRO:HD2  | 1.84                     | 0.58              |
| 39:RT:102:ILE:HB   | 39:RT:110:ILE:HD11 | 1.84                     | 0.58              |
| 41:RV:41:GLY:H     | 41:RV:46:VAL:HG13  | 1.66                     | 0.58              |
| 50:R4:12:ALA:CB    | 50:R4:29:PRO:HA    | 2.33                     | 0.58              |
| 50:R4:42:PHE:CG    | 50:R4:43:TYR:N     | 2.71                     | 0.58              |
| 50:R4:63:TYR:C     | 50:R4:65:ASP:N     | 2.61                     | 0.58              |
| 1:XA:950:U:H2'     | 1:XA:951:G:H8      | 1.68                     | 0.58              |
| 2:XB:212:GLN:NE2   | 2:XB:235:SER:HB2   | 2.18                     | 0.58              |
| 9:XI:114:TYR:O     | 9:XI:114:TYR:HD2   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:13:HIS:HB3   | 10:XJ:68:HIS:CE1   | 2.37                     | 0.58              |
| 11:XK:34:ASP:HB3   | 11:XK:40:ILE:HD11  | 1.83                     | 0.58              |
| 13:XM:19:LEU:HD22  | 13:XM:19:LEU:H     | 1.68                     | 0.58              |
| 25:YA:620:G:H4'    | 25:YA:621:A:C5'    | 2.32                     | 0.58              |
| 25:YA:1354:A:OP1   | 27:YD:38:LYS:HE2   | 2.03                     | 0.58              |
| 28:YE:61:ARG:HB2   | 28:YE:62:PRO:CD    | 2.33                     | 0.58              |
| 28:YE:134:ILE:C    | 28:YE:134:ILE:HD12 | 2.28                     | 0.58              |
| 30:YG:16:ARG:HB3   | 30:YG:17:PRO:CD    | 2.33                     | 0.58              |
| 37:YR:63:ARG:HH11  | 37:YR:63:ARG:HG3   | 1.68                     | 0.58              |
| 42:YW:80:PRO:O     | 42:YW:100:THR:HG22 | 2.03                     | 0.58              |
| 5:QE:79:GLU:OE2    | 8:QH:104:ARG:HA    | 2.03                     | 0.58              |
| 14:QN:23:ARG:CZ    | 14:QN:30:ALA:HB2   | 2.32                     | 0.58              |
| 20:QT:37:SER:HB3   | 20:QT:84:LEU:HD23  | 1.85                     | 0.58              |
| 25:RA:1636:C:H2'   | 25:RA:1637:A:C8    | 2.38                     | 0.58              |
| 29:RF:63:LYS:HE2   | 29:RF:67:GLN:CB    | 2.32                     | 0.58              |
| 44:RY:81:LYS:HD3   | 44:RY:97:ARG:CD    | 2.34                     | 0.58              |
| 48:R2:17:SER:CB    | 48:R2:18:PRO:HA    | 2.33                     | 0.58              |
| 48:R2:69:ARG:NH1   | 48:R2:69:ARG:CB    | 2.67                     | 0.58              |
| 1:XA:690:G:H2'     | 1:XA:691:G:O4'     | 2.04                     | 0.58              |
| 1:XA:1348:U:H4'    | 9:XI:120:ARG:HD2   | 1.84                     | 0.58              |
| 2:XB:80:ILE:HG21   | 2:XB:212:GLN:HA    | 1.84                     | 0.58              |
| 3:XC:181:ASN:HD22  | 3:XC:204:LEU:HB2   | 1.68                     | 0.58              |
| 9:XI:79:LEU:O      | 9:XI:82:ALA:HB3    | 2.02                     | 0.58              |
| 13:XM:66:LEU:O     | 13:XM:67:GLU:C     | 2.46                     | 0.58              |
| 14:XN:21:TYR:HE2   | 14:XN:23:ARG:HH21  | 1.51                     | 0.58              |
| 27:YD:44:ASN:HB3   | 27:YD:49:ILE:CA    | 2.27                     | 0.58              |
| 31:YH:92:ILE:HG22  | 31:YH:93:GLY:N     | 2.18                     | 0.58              |
| 35:YP:37:GLY:C     | 35:YP:41:ARG:HD3   | 2.29                     | 0.58              |
| 35:YP:37:GLY:HA2   | 35:YP:41:ARG:HE    | 1.68                     | 0.58              |
| 36:YQ:66:ILE:HA    | 36:YQ:104:PHE:HA   | 1.85                     | 0.58              |
| 39:YT:36:GLU:HG3   | 39:YT:41:ARG:HD3   | 1.85                     | 0.58              |
| 7:QG:85:TYR:HE1    | 7:QG:154:TYR:CE1   | 2.21                     | 0.58              |
| 8:QH:10:LEU:H      | 8:QH:10:LEU:CD2    | 2.15                     | 0.58              |
| 9:QI:79:LEU:O      | 9:QI:82:ALA:HB3    | 2.03                     | 0.58              |
| 16:QP:28:ARG:HH11  | 16:QP:28:ARG:HG2   | 1.68                     | 0.58              |
| 18:QR:36:ASN:O     | 18:QR:36:ASN:ND2   | 2.32                     | 0.58              |
| 25:RA:270(R):G:H2' | 25:RA:270(S):G:C8  | 2.38                     | 0.58              |
| 25:RA:1266:G:C5    | 42:RW:15:ARG:NH1   | 2.71                     | 0.58              |
| 25:RA:1449:A:HO2'  | 25:RA:1530:G:H21   | 1.49                     | 0.58              |
| 25:RA:2295:C:OP1   | 38:RS:10:ARG:HD2   | 2.03                     | 0.58              |
| 27:RD:242:ARG:HD2  | 27:RD:242:ARG:N    | 2.18                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:6:GLY:HA3    | 28:RE:26:ILE:HD11  | 1.85                     | 0.58              |
| 29:RF:174:VAL:HG13 | 29:RF:174:VAL:O    | 2.03                     | 0.58              |
| 29:RF:179:GLU:CD   | 29:RF:179:GLU:H    | 2.12                     | 0.58              |
| 30:RG:35:GLU:CD    | 30:RG:35:GLU:C     | 2.71                     | 0.58              |
| 31:RH:86:GLU:O     | 31:RH:131:VAL:O    | 2.21                     | 0.58              |
| 34:RO:20:MET:O     | 34:RO:41:ALA:HB1   | 2.04                     | 0.58              |
| 39:RT:88:ILE:C     | 39:RT:88:ILE:HD12  | 2.28                     | 0.58              |
| 40:RU:92:ARG:NH1   | 40:RU:95:LEU:CD1   | 2.65                     | 0.58              |
| 48:R2:16:LEU:O     | 48:R2:16:LEU:CG    | 2.49                     | 0.58              |
| 48:R2:16:LEU:O     | 48:R2:17:SER:HB3   | 2.04                     | 0.58              |
| 51:R5:60:VAL:HG13  | 51:R5:60:VAL:OXT   | 2.03                     | 0.58              |
| 1:XA:864:A:H5'     | 5:XE:86:ALA:HB2    | 1.85                     | 0.58              |
| 5:XE:102:ALA:HB2   | 5:XE:120:THR:OG1   | 2.03                     | 0.58              |
| 9:XI:40:LEU:HD11   | 9:XI:70:LYS:HG2    | 1.84                     | 0.58              |
| 9:XI:127:LYS:NZ    | 22:XV:34:C:OP2     | 2.37                     | 0.58              |
| 12:XL:18:VAL:O     | 12:XL:19:ARG:HB2   | 2.03                     | 0.58              |
| 13:XM:57:ARG:HH11  | 13:XM:57:ARG:CB    | 2.13                     | 0.58              |
| 14:XN:44:LEU:HD13  | 14:XN:53:LEU:HD13  | 1.84                     | 0.58              |
| 25:YA:551:G:H5'    | 25:YA:1220:A:H1'   | 1.84                     | 0.58              |
| 27:YD:165:ILE:HA   | 27:YD:175:LEU:HD23 | 1.83                     | 0.58              |
| 35:YP:65:ARG:HH21  | 54:Y8:15:LYS:CB    | 2.17                     | 0.58              |
| 35:YP:71:VAL:HG13  | 35:YP:72:PRO:HD3   | 1.84                     | 0.58              |
| 37:YR:2:ARG:HG2    | 37:YR:5:LYS:HZ1    | 1.68                     | 0.58              |
| 48:Y2:51:ARG:HA    | 48:Y2:54:LYS:HB2   | 1.86                     | 0.58              |
| 1:QA:1118:C:H1'    | 1:QA:1179:A:C4     | 2.37                     | 0.58              |
| 3:QC:77:ILE:O      | 3:QC:84:ILE:HG22   | 2.02                     | 0.58              |
| 4:QD:196:LEU:O     | 4:QD:198:VAL:N     | 2.31                     | 0.58              |
| 6:QF:97:PHE:O      | 18:QR:31:LEU:HD23  | 2.04                     | 0.58              |
| 7:QG:49:ILE:O      | 7:QG:53:LYS:HB3    | 2.04                     | 0.58              |
| 25:RA:389:G:H1     | 35:RP:71:VAL:HG12  | 1.69                     | 0.58              |
| 25:RA:458:G:O2'    | 25:RA:469:G:O6     | 2.20                     | 0.58              |
| 25:RA:1266:G:O5'   | 42:RW:15:ARG:NH2   | 2.37                     | 0.58              |
| 33:RN:14:VAL:HG12  | 33:RN:15:LEU:N     | 2.19                     | 0.58              |
| 34:RO:71:ARG:HH11  | 34:RO:71:ARG:HG3   | 1.69                     | 0.58              |
| 40:RU:47:TYR:C     | 40:RU:47:TYR:CD2   | 2.81                     | 0.58              |
| 42:RW:95:ILE:HD12  | 42:RW:95:ILE:O     | 2.04                     | 0.58              |
| 44:RY:96:ILE:CD1   | 44:RY:98:VAL:HG12  | 2.33                     | 0.58              |
| 50:R4:15:ILE:HG22  | 50:R4:19:GLY:O     | 2.03                     | 0.58              |
| 50:R4:48:ARG:NH1   | 50:R4:52:THR:H     | 2.01                     | 0.58              |
| 54:R8:46:ARG:O     | 54:R8:47:LYS:HB3   | 2.03                     | 0.58              |
| 1:XA:96:G:H2'      | 1:XA:97:U:O4'      | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:674:G:H2'    | 1:XA:675:A:C8     | 2.38                     | 0.58              |
| 2:XB:47:THR:HG22  | 2:XB:51:LEU:HG    | 1.85                     | 0.58              |
| 12:XL:45:PRO:HD3  | 12:XL:51:ALA:O    | 2.04                     | 0.58              |
| 12:XL:82:VAL:HG23 | 12:XL:106:ASP:OD2 | 2.04                     | 0.58              |
| 13:XM:45:VAL:HG22 | 13:XM:45:VAL:O    | 2.02                     | 0.58              |
| 25:YA:2372:G:H4'  | 52:Y6:46:HIS:NE2  | 2.18                     | 0.58              |
| 28:YE:78:LEU:HD23 | 28:YE:79:ARG:HD2  | 1.86                     | 0.58              |
| 30:YG:64:THR:HG23 | 30:YG:66:GLN:H    | 1.67                     | 0.58              |
| 33:YN:70:LYS:C    | 33:YN:71:ILE:HD13 | 2.28                     | 0.58              |
| 34:YO:40:VAL:HG12 | 34:YO:41:ALA:N    | 2.19                     | 0.58              |
| 35:YP:71:VAL:CG1  | 35:YP:72:PRO:HD3  | 2.33                     | 0.58              |
| 42:YW:66:GLU:O    | 42:YW:68:ARG:N    | 2.33                     | 0.58              |
| 50:Y4:65:ASP:O    | 50:Y4:66:SER:CB   | 2.51                     | 0.58              |
| 5:QE:78:HIS:CE1   | 5:QE:143:ARG:H    | 2.20                     | 0.58              |
| 12:QL:33:ARG:O    | 12:QL:85:ILE:HG22 | 2.03                     | 0.58              |
| 14:QN:23:ARG:H    | 14:QN:33:VAL:HG11 | 1.67                     | 0.58              |
| 18:QR:25:THR:C    | 18:QR:26:LEU:HD23 | 2.29                     | 0.58              |
| 19:QS:40:ILE:HD11 | 19:QS:62:ILE:HG21 | 1.85                     | 0.58              |
| 25:RA:443:A:C5    | 29:RF:45:ARG:HD2  | 2.38                     | 0.58              |
| 25:RA:2723:C:H5'' | 37:RR:1:MET:HG2   | 1.85                     | 0.58              |
| 25:RA:2758:A:C5   | 31:RH:67:LEU:HD21 | 2.39                     | 0.58              |
| 27:RD:34:VAL:C    | 27:RD:35:LYS:HG3  | 2.29                     | 0.58              |
| 29:RF:160:ASN:OD1 | 29:RF:162:LEU:HB2 | 2.04                     | 0.58              |
| 30:RG:16:ARG:NH2  | 30:RG:31:VAL:HG11 | 2.17                     | 0.58              |
| 31:RH:159:GLU:O   | 31:RH:160:LYS:HG2 | 2.02                     | 0.58              |
| 33:RN:70:LYS:C    | 33:RN:71:ILE:HD13 | 2.28                     | 0.58              |
| 36:RQ:81:VAL:C    | 36:RQ:82:ARG:CG   | 2.76                     | 0.58              |
| 40:RU:92:ARG:HH11 | 40:RU:95:LEU:HD12 | 1.67                     | 0.58              |
| 2:XB:115:LEU:HD23 | 2:XB:153:ARG:HD3  | 1.84                     | 0.58              |
| 3:XC:77:ILE:O     | 3:XC:84:ILE:HG22  | 2.02                     | 0.58              |
| 5:XE:68:GLU:O     | 5:XE:68:GLU:HG3   | 2.03                     | 0.58              |
| 8:XH:84:ARG:NH1   | 8:XH:86:ILE:HD13  | 2.11                     | 0.58              |
| 25:YA:2283:C:P    | 52:Y6:5:VAL:HG13  | 2.44                     | 0.58              |
| 28:YE:51:PHE:CD1  | 28:YE:52:LEU:HG   | 2.38                     | 0.58              |
| 29:YF:89:VAL:HG12 | 29:YF:90:PHE:N    | 2.18                     | 0.58              |
| 31:YH:117:PRO:HB3 | 31:YH:123:PHE:CD1 | 2.37                     | 0.58              |
| 36:YQ:55:VAL:HG22 | 36:YQ:56:ARG:N    | 2.18                     | 0.58              |
| 39:YT:88:ILE:C    | 39:YT:88:ILE:HD12 | 2.29                     | 0.58              |
| 41:YV:38:LEU:HD23 | 41:YV:39:LEU:N    | 2.19                     | 0.58              |
| 43:YX:36:LYS:HE3  | 43:YX:54:VAL:O    | 2.04                     | 0.58              |
| 44:YY:51:VAL:CG1  | 44:YY:52:SER:H    | 2.11                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:QD:156:GLU:O    | 4:QD:160:GLN:HG3   | 2.03                     | 0.58              |
| 13:QM:66:LEU:O    | 13:QM:67:GLU:C     | 2.46                     | 0.58              |
| 14:QN:23:ARG:O    | 14:QN:24:CYS:C     | 2.46                     | 0.58              |
| 25:RA:2116:G:N1   | 25:RA:2162:G:OP1   | 2.36                     | 0.58              |
| 27:RD:35:LYS:CG   | 27:RD:64:ILE:H     | 2.15                     | 0.58              |
| 28:RE:51:PHE:CD1  | 28:RE:52:LEU:HG    | 2.38                     | 0.58              |
| 31:RH:4:ILE:HG13  | 31:RH:6:ARG:CD     | 2.33                     | 0.58              |
| 1:XA:1320:C:N4    | 19:XS:36:ARG:HG3   | 2.18                     | 0.58              |
| 2:XB:75:LYS:HD3   | 2:XB:75:LYS:C      | 2.29                     | 0.58              |
| 3:XC:36:ASP:HB3   | 3:XC:40:ARG:HH12   | 1.68                     | 0.58              |
| 3:XC:189:ALA:HB3  | 3:XC:196:LEU:HB2   | 1.84                     | 0.58              |
| 4:XD:191:ARG:NH1  | 4:XD:200:GLU:OE1   | 2.37                     | 0.58              |
| 7:XG:49:ILE:O     | 7:XG:53:LYS:HB3    | 2.03                     | 0.58              |
| 13:XM:65:LYS:HE2  | 50:Y4:50:VAL:HG11  | 1.86                     | 0.58              |
| 16:XP:14:ASN:N    | 16:XP:15:PRO:CD    | 2.67                     | 0.58              |
| 16:XP:53:VAL:HG23 | 16:XP:54:GLU:N     | 2.17                     | 0.58              |
| 25:YA:451:C:H4'   | 29:YF:52:LYS:HZ2   | 1.68                     | 0.58              |
| 25:YA:1138:G:H21  | 33:YN:106:MET:HE3  | 1.69                     | 0.58              |
| 25:YA:1543:A:O2'  | 25:YA:1544:C:H3'   | 2.04                     | 0.58              |
| 25:YA:2563:U:H4'  | 34:YO:28:SER:HA    | 1.85                     | 0.58              |
| 25:YA:2636:U:OP1  | 28:YE:79:ARG:HA    | 2.04                     | 0.58              |
| 27:YD:34:VAL:C    | 27:YD:35:LYS:HG3   | 2.28                     | 0.58              |
| 29:YF:138:GLU:O   | 29:YF:141:ALA:HB3  | 2.03                     | 0.58              |
| 31:YH:85:LYS:HA   | 31:YH:86:GLU:OE1   | 2.04                     | 0.58              |
| 33:YN:9:VAL:HG21  | 33:YN:48:MET:HB3   | 1.85                     | 0.58              |
| 34:YO:7:TYR:C     | 34:YO:8:LEU:HD22   | 2.29                     | 0.58              |
| 34:YO:12:ASP:CG   | 34:YO:14:THR:HG23  | 2.29                     | 0.58              |
| 42:YW:95:ILE:HD12 | 42:YW:95:ILE:O     | 2.04                     | 0.58              |
| 43:YX:7:VAL:O     | 43:YX:30:VAL:HG12  | 2.04                     | 0.58              |
| 48:Y2:17:SER:CB   | 48:Y2:18:PRO:HA    | 2.33                     | 0.58              |
| 3:QC:105:GLU:HG2  | 3:QC:106:VAL:N     | 2.18                     | 0.58              |
| 4:QD:22:LYS:O     | 4:QD:113:SER:HB3   | 2.03                     | 0.58              |
| 10:QJ:3:LYS:O     | 10:QJ:100:THR:HG22 | 2.04                     | 0.58              |
| 13:QM:56:LEU:HD13 | 13:QM:60:VAL:HG23  | 1.86                     | 0.58              |
| 16:QP:51:VAL:CG1  | 16:QP:52:ASP:N     | 2.65                     | 0.58              |
| 16:QP:75:ARG:C    | 16:QP:77:ALA:H     | 2.11                     | 0.58              |
| 25:RA:2693:A:H2'  | 25:RA:2694:G:C8    | 2.36                     | 0.58              |
| 29:RF:11:VAL:HG11 | 29:RF:18:ARG:HE    | 1.67                     | 0.58              |
| 34:RO:12:ASP:CG   | 34:RO:14:THR:HG23  | 2.29                     | 0.58              |
| 35:RP:37:GLY:C    | 35:RP:41:ARG:HD3   | 2.29                     | 0.58              |
| 38:RS:67:ARG:HB2  | 38:RS:67:ARG:HH11  | 1.65                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RX:7:VAL:O      | 43:RX:30:VAL:HG12  | 2.04                     | 0.58              |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:H    | 1.69                     | 0.58              |
| 54:R8:56:GLU:O     | 54:R8:59:LYS:N     | 2.35                     | 0.58              |
| 2:XB:140:HIS:HA    | 2:XB:143:GLU:OE1   | 2.04                     | 0.58              |
| 3:XC:95:THR:HG22   | 3:XC:96:GLY:N      | 2.07                     | 0.58              |
| 12:XL:54:LYS:N     | 12:XL:54:LYS:HD2   | 2.18                     | 0.58              |
| 16:XP:28:ARG:HH11  | 16:XP:28:ARG:HG2   | 1.68                     | 0.58              |
| 25:YA:2636:U:H1'   | 25:YA:2783:G:N2    | 2.19                     | 0.58              |
| 27:YD:242:ARG:HD2  | 27:YD:242:ARG:N    | 2.18                     | 0.58              |
| 28:YE:72:VAL:O     | 28:YE:73:GLU:O     | 2.21                     | 0.58              |
| 29:YF:179:GLU:CD   | 29:YF:179:GLU:H    | 2.11                     | 0.58              |
| 35:YP:112:LEU:HD13 | 35:YP:112:LEU:C    | 2.29                     | 0.58              |
| 36:YQ:47:ILE:CD1   | 36:YQ:70:PRO:HD3   | 2.34                     | 0.58              |
| 38:YS:67:ARG:NH1   | 38:YS:67:ARG:CB    | 2.64                     | 0.58              |
| 40:YU:47:TYR:C     | 40:YU:47:TYR:CD2   | 2.81                     | 0.58              |
| 48:Y2:69:ARG:NH1   | 48:Y2:69:ARG:CB    | 2.67                     | 0.58              |
| 50:Y4:12:ALA:CB    | 50:Y4:29:PRO:HA    | 2.33                     | 0.58              |
| 1:QA:1321:C:H5''   | 1:QA:1322:C:H5''   | 1.86                     | 0.58              |
| 2:QB:21:ARG:HG3    | 2:QB:38:GLY:O      | 2.01                     | 0.58              |
| 2:QB:212:GLN:NE2   | 2:QB:235:SER:HB2   | 2.18                     | 0.58              |
| 7:QG:69:VAL:HG11   | 7:QG:104:LEU:CD2   | 2.33                     | 0.58              |
| 12:QL:10:LEU:CD1   | 17:QQ:32:TYR:CE2   | 2.82                     | 0.58              |
| 13:QM:19:LEU:HD22  | 13:QM:19:LEU:H     | 1.68                     | 0.58              |
| 13:QM:81:LEU:HB3   | 13:QM:89:GLY:CA    | 2.34                     | 0.58              |
| 17:QQ:32:TYR:O     | 17:QQ:34:LYS:N     | 2.37                     | 0.58              |
| 19:QS:17:GLU:HA    | 19:QS:20:LEU:HD12  | 1.86                     | 0.58              |
| 25:RA:64:A:C4      | 43:RX:66:LEU:HD13  | 2.39                     | 0.58              |
| 25:RA:1224:G:OP2   | 41:RV:66:ARG:NH2   | 2.37                     | 0.58              |
| 27:RD:27:THR:CG2   | 27:RD:83:GLU:HB3   | 2.33                     | 0.58              |
| 28:RE:111:ARG:NE   | 28:RE:160:TYR:HE1  | 2.01                     | 0.58              |
| 28:RE:134:ILE:C    | 28:RE:134:ILE:HD12 | 2.28                     | 0.58              |
| 29:RF:53:THR:C     | 29:RF:55:GLY:H     | 2.11                     | 0.58              |
| 37:RR:117:VAL:CG2  | 37:RR:118:GLU:H    | 2.15                     | 0.58              |
| 43:RX:27:THR:HB    | 43:RX:80:ILE:HB    | 1.84                     | 0.58              |
| 44:RY:95:LYS:HD3   | 44:RY:95:LYS:H     | 1.68                     | 0.58              |
| 50:R4:3:GLU:HG3    | 50:R4:4:GLY:N      | 2.19                     | 0.58              |
| 50:R4:22:ILE:HG22  | 50:R4:23:GLU:N     | 2.18                     | 0.58              |
| 51:R5:50:GLY:O     | 51:R5:51:TYR:HB2   | 2.03                     | 0.58              |
| 2:XB:19:HIS:NE2    | 2:XB:206:ASP:HB2   | 2.18                     | 0.58              |
| 2:XB:111:ARG:HA    | 2:XB:111:ARG:NE    | 2.18                     | 0.58              |
| 3:XC:76:VAL:HG21   | 3:XC:103:VAL:CG1   | 2.34                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:XI:17:VAL:HG13   | 9:XI:81:ILE:HD13  | 1.85                     | 0.58              |
| 25:YA:200:U:O2     | 25:YA:386:G:N2    | 2.36                     | 0.58              |
| 25:YA:222:A:H62    | 25:YA:232:G:N2    | 2.02                     | 0.58              |
| 25:YA:593:G:H2'    | 25:YA:594:U:C6    | 2.38                     | 0.58              |
| 25:YA:993:G:OP1    | 40:YU:50:ARG:NH2  | 2.35                     | 0.58              |
| 28:YE:63:LEU:HD13  | 28:YE:65:GLY:H    | 1.68                     | 0.58              |
| 28:YE:111:ARG:NE   | 28:YE:160:TYR:HE1 | 2.01                     | 0.58              |
| 33:YN:13:TRP:O     | 33:YN:135:PRO:HD2 | 2.03                     | 0.58              |
| 33:YN:35:ARG:O     | 33:YN:37:LYS:N    | 2.37                     | 0.58              |
| 41:YV:81:TYR:C     | 41:YV:82:ARG:HG3  | 2.27                     | 0.58              |
| 1:QA:538:G:OP1     | 12:QL:113:ARG:HD2 | 2.04                     | 0.58              |
| 1:QA:919:A:O2'     | 1:QA:1080:A:N1    | 2.36                     | 0.58              |
| 2:QB:75:LYS:HD3    | 2:QB:75:LYS:C     | 2.29                     | 0.58              |
| 16:QP:21:VAL:HG22  | 16:QP:34:GLU:O    | 2.04                     | 0.58              |
| 25:RA:194:G:H2'    | 25:RA:195:A:O4'   | 2.04                     | 0.58              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CG  | 2.34                     | 0.58              |
| 31:RH:153:LYS:HA   | 31:RH:153:LYS:HZ3 | 1.68                     | 0.58              |
| 35:RP:71:VAL:CG1   | 35:RP:72:PRO:HD3  | 2.33                     | 0.58              |
| 36:RQ:47:ILE:CD1   | 36:RQ:70:PRO:HD3  | 2.34                     | 0.58              |
| 40:RU:24:TYR:HE1   | 40:RU:39:LEU:HD23 | 1.69                     | 0.58              |
| 41:RV:81:TYR:C     | 41:RV:82:ARG:HG3  | 2.27                     | 0.58              |
| 42:RW:43:GLY:O     | 42:RW:44:ALA:C    | 2.46                     | 0.58              |
| 48:R2:15:LYS:H     | 48:R2:67:LYS:NZ   | 2.02                     | 0.58              |
| 50:R4:27:THR:O     | 50:R4:28:LYS:HB3  | 2.04                     | 0.58              |
| 1:XA:1346:A:C5'    | 9:XI:120:ARG:HH12 | 2.17                     | 0.58              |
| 3:XC:33:LEU:O      | 3:XC:37:GLN:HG2   | 2.04                     | 0.58              |
| 7:XG:69:VAL:HG11   | 7:XG:104:LEU:CD2  | 2.34                     | 0.58              |
| 25:YA:227:A:OP1    | 35:YP:76:LYS:HE3  | 2.04                     | 0.58              |
| 25:YA:566:U:OP1    | 35:YP:29:LYS:HE2  | 2.03                     | 0.58              |
| 25:YA:1228:G:OP2   | 40:YU:16:LYS:NZ   | 2.30                     | 0.58              |
| 26:YB:12:C:O2'     | 46:Y0:74:ARG:HG3  | 2.04                     | 0.58              |
| 29:YF:160:ASN:OD1  | 29:YF:162:LEU:HB2 | 2.04                     | 0.58              |
| 30:YG:39:ILE:HG23  | 30:YG:155:MET:HG3 | 1.86                     | 0.58              |
| 31:YH:4:ILE:HD13   | 31:YH:4:ILE:H     | 1.68                     | 0.58              |
| 38:YS:95:HIS:CG    | 38:YS:96:GLY:H    | 2.21                     | 0.58              |
| 41:YV:78:LYS:O     | 41:YV:79:VAL:HB   | 2.03                     | 0.58              |
| 42:YW:43:GLY:O     | 42:YW:44:ALA:C    | 2.46                     | 0.58              |
| 43:YX:27:THR:HB    | 43:YX:80:ILE:HB   | 1.84                     | 0.58              |
| 44:YY:81:LYS:HD3   | 44:YY:97:ARG:CD   | 2.34                     | 0.58              |
| 48:Y2:15:LYS:H     | 48:Y2:67:LYS:CE   | 2.17                     | 0.58              |
| 49:Y3:22:ALA:O     | 49:Y3:25:ALA:HB3  | 2.04                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Y5:60:VAL:HG13  | 51:Y5:60:VAL:OXT   | 2.03                     | 0.58              |
| 1:QA:1158:C:H4'    | 2:QB:133:LYS:HZ1   | 1.68                     | 0.57              |
| 1:QA:1346:A:C5'    | 9:QI:120:ARG:HH12  | 2.17                     | 0.57              |
| 3:QC:181:ASN:HD22  | 3:QC:204:LEU:HB2   | 1.67                     | 0.57              |
| 11:QK:21:ILE:HG13  | 11:QK:30:VAL:HG12  | 1.86                     | 0.57              |
| 11:QK:30:VAL:HG21  | 11:QK:65:ALA:HA    | 1.85                     | 0.57              |
| 25:RA:373:U:H2'    | 25:RA:374:A:H8     | 1.69                     | 0.57              |
| 25:RA:1049:C:H2'   | 25:RA:1050:A:H5''  | 1.84                     | 0.57              |
| 27:RD:25:THR:HG21  | 27:RD:81:ALA:HB1   | 1.85                     | 0.57              |
| 27:RD:147:LEU:HD13 | 27:RD:155:LEU:CD1  | 2.29                     | 0.57              |
| 30:RG:125:PHE:C    | 30:RG:127:GLY:H    | 2.12                     | 0.57              |
| 31:RH:85:LYS:HA    | 31:RH:86:GLU:OE1   | 2.04                     | 0.57              |
| 35:RP:59:LEU:HA    | 35:RP:61:ARG:CZ    | 2.34                     | 0.57              |
| 39:RT:82:LEU:HD12  | 39:RT:82:LEU:N     | 2.19                     | 0.57              |
| 41:RV:35:LEU:HD21  | 41:RV:57:VAL:CG2   | 2.30                     | 0.57              |
| 45:RZ:58:VAL:O     | 45:RZ:60:GLU:N     | 2.35                     | 0.57              |
| 50:R4:15:ILE:HG22  | 50:R4:20:ASN:HA    | 1.86                     | 0.57              |
| 51:R5:55:ARG:NH1   | 51:R5:58:LEU:HD11  | 2.19                     | 0.57              |
| 8:XH:19:VAL:O      | 8:XH:20:TYR:HB2    | 2.04                     | 0.57              |
| 8:XH:86:ILE:HG13   | 8:XH:133:LEU:HD22  | 1.84                     | 0.57              |
| 12:XL:33:ARG:O     | 12:XL:85:ILE:HG22  | 2.03                     | 0.57              |
| 13:XM:4:ILE:HG22   | 13:XM:5:ALA:N      | 2.19                     | 0.57              |
| 15:XO:4:THR:HB     | 15:XO:6:GLU:OE2    | 2.02                     | 0.57              |
| 27:YD:263:ARG:HB2  | 27:YD:263:ARG:HH11 | 1.67                     | 0.57              |
| 28:YE:6:GLY:HA3    | 28:YE:26:ILE:HD11  | 1.85                     | 0.57              |
| 31:YH:127:GLU:HG2  | 31:YH:128:PRO:CG   | 2.32                     | 0.57              |
| 33:YN:114:ARG:O    | 33:YN:115:ARG:HB3  | 2.03                     | 0.57              |
| 37:YR:117:VAL:CG2  | 37:YR:118:GLU:H    | 2.15                     | 0.57              |
| 46:Y0:27:GLU:HG3   | 46:Y0:68:GLU:HA    | 1.85                     | 0.57              |
| 48:Y2:21:LEU:O     | 48:Y2:25:VAL:HG23  | 2.04                     | 0.57              |
| 2:QB:80:ILE:HG21   | 2:QB:212:GLN:HA    | 1.84                     | 0.57              |
| 2:QB:111:ARG:HA    | 2:QB:111:ARG:NE    | 2.19                     | 0.57              |
| 2:QB:140:HIS:HA    | 2:QB:143:GLU:OE1   | 2.04                     | 0.57              |
| 3:QC:14:ILE:HG12   | 3:QC:15:THR:N      | 2.19                     | 0.57              |
| 5:QE:153:LYS:HB2   | 5:QE:153:LYS:NZ    | 2.18                     | 0.57              |
| 11:QK:32:ILE:O     | 11:QK:40:ILE:HG12  | 2.04                     | 0.57              |
| 17:QQ:84:LEU:C     | 17:QQ:86:GLU:N     | 2.60                     | 0.57              |
| 25:RA:1636:C:H2'   | 25:RA:1637:A:H8    | 1.68                     | 0.57              |
| 27:RD:35:LYS:HG2   | 27:RD:64:ILE:CA    | 2.34                     | 0.57              |
| 29:RF:138:GLU:O    | 29:RF:141:ALA:HB3  | 2.04                     | 0.57              |
| 30:RG:39:ILE:HG23  | 30:RG:155:MET:HG3  | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:84:SER:O     | 31:RH:133:VAL:O    | 2.22                     | 0.57              |
| 31:RH:125:VAL:HA   | 31:RH:126:PRO:CB   | 2.29                     | 0.57              |
| 34:RO:20:MET:HG2   | 34:RO:21:CYS:N     | 2.19                     | 0.57              |
| 35:RP:112:LEU:HD13 | 35:RP:112:LEU:C    | 2.29                     | 0.57              |
| 38:RS:95:HIS:CG    | 38:RS:96:GLY:H     | 2.21                     | 0.57              |
| 38:RS:106:ARG:O    | 38:RS:107:GLU:HB2  | 2.04                     | 0.57              |
| 41:RV:78:LYS:O     | 41:RV:79:VAL:HB    | 2.04                     | 0.57              |
| 42:RW:80:PRO:O     | 42:RW:100:THR:HG22 | 2.03                     | 0.57              |
| 50:R4:39:CYS:O     | 50:R4:40:HIS:HB2   | 2.03                     | 0.57              |
| 2:XB:12:GLU:O      | 2:XB:16:HIS:ND1    | 2.36                     | 0.57              |
| 2:XB:106:LYS:O     | 2:XB:110:GLN:HG3   | 2.04                     | 0.57              |
| 4:XD:33:MET:HE2    | 4:XD:37:PRO:HA     | 1.86                     | 0.57              |
| 12:XL:83:VAL:HG22  | 12:XL:84:LEU:H     | 1.70                     | 0.57              |
| 13:XM:3:ARG:HG2    | 50:Y4:34:GLU:OE1   | 2.04                     | 0.57              |
| 20:XT:37:SER:HB3   | 20:XT:84:LEU:HD23  | 1.85                     | 0.57              |
| 25:YA:483:A:C4'    | 44:YY:49:VAL:HA    | 2.29                     | 0.57              |
| 27:YD:35:LYS:HG2   | 27:YD:64:ILE:CA    | 2.34                     | 0.57              |
| 27:YD:71:ASP:HB3   | 27:YD:103:ARG:HH22 | 1.68                     | 0.57              |
| 28:YE:203:LYS:HE3  | 28:YE:204:ALA:HB2  | 1.86                     | 0.57              |
| 29:YF:53:THR:C     | 29:YF:55:GLY:H     | 2.11                     | 0.57              |
| 32:YI:4:ILE:HG12   | 32:YI:18:VAL:HG22  | 1.86                     | 0.57              |
| 39:YT:82:LEU:HD12  | 39:YT:82:LEU:N     | 2.19                     | 0.57              |
| 40:YU:39:LEU:O     | 40:YU:40:PHE:C     | 2.48                     | 0.57              |
| 1:QA:372:C:N4      | 1:QA:389:A:H62     | 2.02                     | 0.57              |
| 2:QB:12:GLU:O      | 2:QB:16:HIS:ND1    | 2.36                     | 0.57              |
| 4:QD:100:ARG:HH22  | 4:QD:137:SER:HB3   | 1.70                     | 0.57              |
| 25:RA:2146:C:H4'   | 25:RA:2147:G:C8    | 2.39                     | 0.57              |
| 27:RD:177:LEU:HD11 | 27:RD:183:ARG:HB2  | 1.85                     | 0.57              |
| 27:RD:263:ARG:HB2  | 27:RD:263:ARG:HH11 | 1.67                     | 0.57              |
| 29:RF:29:ASN:N     | 29:RF:112:MET:HE1  | 2.19                     | 0.57              |
| 32:RI:62:LYS:HE3   | 32:RI:134:PRO:HG2  | 1.86                     | 0.57              |
| 36:RQ:55:VAL:HG22  | 36:RQ:56:ARG:N     | 2.18                     | 0.57              |
| 38:RS:67:ARG:HH11  | 38:RS:67:ARG:CB    | 2.18                     | 0.57              |
| 47:R1:81:LYS:HE2   | 47:R1:81:LYS:H     | 1.62                     | 0.57              |
| 50:R4:37:SER:HB3   | 50:R4:42:PHE:CE1   | 2.38                     | 0.57              |
| 50:R4:38:LYS:C     | 50:R4:40:HIS:H     | 2.07                     | 0.57              |
| 1:XA:17:U:H2'      | 1:XA:18:C:C6       | 2.39                     | 0.57              |
| 4:XD:156:GLU:O     | 4:XD:160:GLN:HG3   | 2.03                     | 0.57              |
| 4:XD:196:LEU:O     | 4:XD:198:VAL:N     | 2.31                     | 0.57              |
| 6:XF:39:LYS:HD2    | 6:XF:64:GLN:NE2    | 2.19                     | 0.57              |
| 7:XG:62:PHE:HA     | 7:XG:124:LEU:CD2   | 2.27                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:XM:84:ILE:HG23 | 13:XM:85:GLY:N    | 2.17                     | 0.57              |
| 22:XV:53:G:H4'    | 22:XV:54:U:OP1    | 2.03                     | 0.57              |
| 25:YA:2635:C:OP1  | 28:YE:78:LEU:HD12 | 2.04                     | 0.57              |
| 28:YE:63:LEU:HD12 | 28:YE:65:GLY:H    | 1.69                     | 0.57              |
| 31:YH:76:VAL:C    | 31:YH:78:GLY:H    | 2.13                     | 0.57              |
| 38:YS:26:LEU:CD2  | 38:YS:87:PHE:HD1  | 2.17                     | 0.57              |
| 50:Y4:37:SER:HB3  | 50:Y4:42:PHE:CE1  | 2.38                     | 0.57              |
| 2:QB:178:ARG:NE   | 8:QH:71:GLY:O     | 2.37                     | 0.57              |
| 3:QC:77:ILE:O     | 3:QC:83:ARG:HB3   | 2.05                     | 0.57              |
| 13:QM:82:MET:O    | 13:QM:84:ILE:N    | 2.38                     | 0.57              |
| 15:QO:6:GLU:CD    | 15:QO:6:GLU:H     | 2.12                     | 0.57              |
| 16:QP:76:GLN:HG2  | 16:QP:76:GLN:O    | 2.04                     | 0.57              |
| 25:RA:1449:A:O2'  | 25:RA:1530:G:N2   | 2.32                     | 0.57              |
| 25:RA:1496:A:H8   | 25:RA:1577:C:HO2' | 1.51                     | 0.57              |
| 25:RA:1509:C:H3'  | 25:RA:1510:A:H5'' | 1.86                     | 0.57              |
| 25:RA:2749:A:H4'  | 31:RH:62:LYS:HB3  | 1.85                     | 0.57              |
| 28:RE:51:PHE:HD1  | 28:RE:52:LEU:HG   | 1.68                     | 0.57              |
| 28:RE:63:LEU:HD13 | 28:RE:65:GLY:H    | 1.68                     | 0.57              |
| 30:RG:16:ARG:HB3  | 30:RG:17:PRO:CD   | 2.33                     | 0.57              |
| 30:RG:63:ILE:HD11 | 30:RG:102:PHE:HE2 | 1.69                     | 0.57              |
| 31:RH:4:ILE:HD13  | 31:RH:4:ILE:H     | 1.69                     | 0.57              |
| 33:RN:35:ARG:O    | 33:RN:37:LYS:N    | 2.37                     | 0.57              |
| 33:RN:42:TRP:O    | 40:RU:64:ARG:NH2  | 2.35                     | 0.57              |
| 34:RO:40:VAL:HG12 | 34:RO:41:ALA:N    | 2.19                     | 0.57              |
| 36:RQ:66:ILE:HA   | 36:RQ:104:PHE:HA  | 1.85                     | 0.57              |
| 37:RR:63:ARG:HH11 | 37:RR:63:ARG:HG3  | 1.68                     | 0.57              |
| 38:RS:26:LEU:CD2  | 38:RS:87:PHE:HD1  | 2.17                     | 0.57              |
| 52:R6:6:ARG:O     | 52:R6:8:LYS:HD2   | 2.05                     | 0.57              |
| 1:XA:356:A:N3     | 1:XA:368:U:O2'    | 2.30                     | 0.57              |
| 2:XB:77:ALA:CB    | 2:XB:211:ILE:HG21 | 2.35                     | 0.57              |
| 3:XC:14:ILE:HG12  | 3:XC:15:THR:N     | 2.19                     | 0.57              |
| 4:XD:13:ARG:O     | 4:XD:16:GLY:N     | 2.29                     | 0.57              |
| 11:XK:21:ILE:HD12 | 11:XK:21:ILE:N    | 2.20                     | 0.57              |
| 15:XO:6:GLU:CD    | 15:XO:6:GLU:H     | 2.12                     | 0.57              |
| 16:XP:76:GLN:O    | 16:XP:76:GLN:HG2  | 2.04                     | 0.57              |
| 19:XS:15:LEU:HD23 | 19:XS:15:LEU:N    | 2.19                     | 0.57              |
| 25:YA:392:C:H5''  | 25:YA:409:C:H5''  | 1.84                     | 0.57              |
| 28:YE:152:LYS:HG2 | 33:YN:78:TYR:CE1  | 2.39                     | 0.57              |
| 30:YG:63:ILE:HD11 | 30:YG:102:PHE:HE2 | 1.69                     | 0.57              |
| 32:YI:2:LYS:HA    | 32:YI:20:ASP:HA   | 1.87                     | 0.57              |
| 33:YN:14:VAL:HG12 | 33:YN:15:LEU:H    | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:YU:24:TYR:HE1  | 40:YU:39:LEU:HD23 | 1.70                     | 0.57              |
| 48:Y2:16:LEU:O    | 48:Y2:17:SER:HB3  | 2.04                     | 0.57              |
| 49:Y3:4:LEU:O     | 49:Y3:36:VAL:HA   | 2.04                     | 0.57              |
| 7:QG:16:LEU:CD1   | 9:QI:45:ALA:HB2   | 2.34                     | 0.57              |
| 10:QJ:64:GLU:OE2  | 10:QJ:66:ARG:HD2  | 2.05                     | 0.57              |
| 12:QL:126:LYS:HB2 | 12:QL:126:LYS:HZ2 | 1.69                     | 0.57              |
| 19:QS:65:ASN:N    | 19:QS:65:ASN:ND2  | 2.52                     | 0.57              |
| 25:RA:607:U:OP1   | 29:RF:102:PRO:HA  | 2.05                     | 0.57              |
| 30:RG:39:ILE:CG2  | 30:RG:155:MET:HG3 | 2.35                     | 0.57              |
| 33:RN:133:GLN:O   | 33:RN:134:ARG:CB  | 2.53                     | 0.57              |
| 34:RO:7:TYR:C     | 34:RO:8:LEU:HD22  | 2.29                     | 0.57              |
| 36:RQ:58:PHE:O    | 36:RQ:59:ARG:C    | 2.43                     | 0.57              |
| 38:RS:103:GLU:O   | 38:RS:106:ARG:CG  | 2.52                     | 0.57              |
| 47:R1:86:SER:H    | 47:R1:87:PRO:CD   | 2.16                     | 0.57              |
| 48:R2:15:LYS:H    | 48:R2:67:LYS:CE   | 2.17                     | 0.57              |
| 48:R2:17:SER:HB2  | 48:R2:18:PRO:HA   | 1.86                     | 0.57              |
| 48:R2:21:LEU:O    | 48:R2:25:VAL:HG23 | 2.04                     | 0.57              |
| 54:R8:53:PRO:CD   | 54:R8:54:GLU:H    | 2.15                     | 0.57              |
| 55:R9:25:VAL:HB   | 55:R9:34:GLN:HB2  | 1.86                     | 0.57              |
| 2:XB:97:TRP:HH2   | 2:XB:176:GLU:HB2  | 1.69                     | 0.57              |
| 6:XF:69:GLU:C     | 6:XF:71:ARG:H     | 2.13                     | 0.57              |
| 7:XG:37:ASN:HD21  | 9:XI:40:LEU:HD23  | 1.69                     | 0.57              |
| 7:XG:121:ALA:O    | 7:XG:125:MET:N    | 2.37                     | 0.57              |
| 11:XK:29:ILE:HG13 | 11:XK:43:SER:O    | 2.05                     | 0.57              |
| 13:XM:81:LEU:HB3  | 13:XM:89:GLY:CA   | 2.34                     | 0.57              |
| 19:XS:42:PRO:HD3  | 50:Y4:63:TYR:HE2  | 1.69                     | 0.57              |
| 25:YA:389:G:H22   | 35:YP:72:PRO:CG   | 2.16                     | 0.57              |
| 25:YA:2250:G:C2   | 36:YQ:82:ARG:HB3  | 2.39                     | 0.57              |
| 25:YA:2286:A:H2'  | 52:Y6:31:PRO:HG2  | 1.87                     | 0.57              |
| 25:YA:2729:G:H1'  | 28:YE:187:ALA:HB2 | 1.87                     | 0.57              |
| 28:YE:116:VAL:CG2 | 28:YE:122:PHE:CD2 | 2.86                     | 0.57              |
| 33:YN:14:VAL:HG12 | 33:YN:15:LEU:N    | 2.18                     | 0.57              |
| 34:YO:20:MET:O    | 34:YO:41:ALA:HB1  | 2.04                     | 0.57              |
| 38:YS:5:THR:HG23  | 38:YS:8:GLU:OE2   | 2.04                     | 0.57              |
| 38:YS:72:ALA:O    | 38:YS:76:LYS:HG3  | 2.04                     | 0.57              |
| 38:YS:106:ARG:O   | 38:YS:107:GLU:HB2 | 2.04                     | 0.57              |
| 47:Y1:86:SER:H    | 47:Y1:87:PRO:CD   | 2.16                     | 0.57              |
| 51:Y5:50:GLY:O    | 51:Y5:51:TYR:HB2  | 2.02                     | 0.57              |
| 1:QA:128:G:O2'    | 17:QQ:3:LYS:NZ    | 2.37                     | 0.57              |
| 1:QA:1259:C:N4    | 1:QA:1260:C:O2    | 2.38                     | 0.57              |
| 2:QB:97:TRP:HH2   | 2:QB:176:GLU:HB2  | 1.69                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:QC:57:ILE:HG23   | 3:QC:64:VAL:HG13   | 1.86                     | 0.57              |
| 3:QC:90:GLU:O      | 3:QC:94:LEU:HG     | 2.05                     | 0.57              |
| 4:QD:50:ARG:O      | 4:QD:50:ARG:HD2    | 2.05                     | 0.57              |
| 4:QD:191:ARG:NH1   | 4:QD:200:GLU:OE1   | 2.37                     | 0.57              |
| 11:QK:69:ALA:HB1   | 11:QK:103:LEU:HD21 | 1.85                     | 0.57              |
| 18:QR:85:LEU:HD23  | 18:QR:88:LYS:HD2   | 1.86                     | 0.57              |
| 20:QT:10:LEU:HG    | 20:QT:12:ALA:H     | 1.70                     | 0.57              |
| 25:RA:298:G:O2'    | 25:RA:322:A:N1     | 2.32                     | 0.57              |
| 25:RA:1279:G:H4'   | 37:RR:31:HIS:HD2   | 1.69                     | 0.57              |
| 25:RA:2839:G:H21   | 37:RR:92:GLY:HA3   | 1.68                     | 0.57              |
| 28:RE:74:PRO:HG2   | 28:RE:77:ILE:HG23  | 1.86                     | 0.57              |
| 30:RG:107:LEU:HD11 | 30:RG:178:PHE:CE1  | 2.39                     | 0.57              |
| 31:RH:76:VAL:C     | 31:RH:78:GLY:H     | 2.13                     | 0.57              |
| 32:RI:129:THR:HA   | 32:RI:137:PRO:HA   | 1.87                     | 0.57              |
| 33:RN:40:PRO:HB3   | 40:RU:68:ALA:HB2   | 1.86                     | 0.57              |
| 49:R3:22:ALA:O     | 49:R3:25:ALA:HB3   | 2.04                     | 0.57              |
| 1:XA:626:U:H2'     | 1:XA:627:G:C8      | 2.39                     | 0.57              |
| 1:XA:1069:C:O2'    | 5:XE:25:ARG:NH1    | 2.36                     | 0.57              |
| 5:XE:140:ARG:HH11  | 5:XE:140:ARG:CB    | 2.17                     | 0.57              |
| 5:XE:140:ARG:HH11  | 5:XE:140:ARG:HB2   | 1.69                     | 0.57              |
| 13:XM:65:LYS:HZ1   | 50:Y4:52:THR:HG21  | 1.68                     | 0.57              |
| 15:XO:8:LYS:HB2    | 15:XO:8:LYS:HZ2    | 1.69                     | 0.57              |
| 16:XP:75:ARG:C     | 16:XP:77:ALA:H     | 2.11                     | 0.57              |
| 25:YA:1434:A:H61   | 25:YA:1558:A:H62   | 1.52                     | 0.57              |
| 25:YA:2033:A:O2'   | 25:YA:2035:G:OP2   | 2.23                     | 0.57              |
| 25:YA:2695:C:H2'   | 25:YA:2696:U:C6    | 2.40                     | 0.57              |
| 27:YD:28:GLU:O     | 27:YD:29:PRO:C     | 2.45                     | 0.57              |
| 28:YE:41:LYS:HE2   | 28:YE:41:LYS:HA    | 1.87                     | 0.57              |
| 30:YG:107:LEU:HD11 | 30:YG:178:PHE:CE1  | 2.40                     | 0.57              |
| 31:YH:3:ARG:HA     | 31:YH:3:ARG:HE     | 1.69                     | 0.57              |
| 33:YN:133:GLN:O    | 33:YN:134:ARG:CB   | 2.53                     | 0.57              |
| 34:YO:71:ARG:HG3   | 34:YO:71:ARG:HH11  | 1.69                     | 0.57              |
| 37:YR:32:GLY:O     | 37:YR:115:GLU:HA   | 2.04                     | 0.57              |
| 37:YR:56:LYS:C     | 37:YR:58:GLY:N     | 2.61                     | 0.57              |
| 40:YU:52:ARG:HG2   | 40:YU:52:ARG:NH1   | 2.18                     | 0.57              |
| 51:Y5:55:ARG:NH1   | 51:Y5:58:LEU:HD11  | 2.19                     | 0.57              |
| 6:QF:39:LYS:HD2    | 6:QF:64:GLN:NE2    | 2.19                     | 0.57              |
| 6:QF:99:ALA:O      | 6:QF:100:ASN:HB2   | 2.04                     | 0.57              |
| 14:QN:13:THR:N     | 14:QN:14:PRO:CD    | 2.68                     | 0.57              |
| 25:RA:78:A:H2'     | 25:RA:79:G:H8      | 1.69                     | 0.57              |
| 25:RA:857:C:OP2    | 46:R0:77:ARG:NH2   | 2.37                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1266:G:OP2   | 51:R5:20:ARG:NE    | 2.37                     | 0.57              |
| 31:RH:124:GLU:HB3  | 31:RH:132:ARG:HG3  | 1.85                     | 0.57              |
| 32:RI:30:LEU:HB3   | 32:RI:36:ALA:HB3   | 1.85                     | 0.57              |
| 33:RN:7:LYS:HG2    | 33:RN:8:GLN:N      | 2.20                     | 0.57              |
| 37:RR:32:GLY:O     | 37:RR:115:GLU:HA   | 2.04                     | 0.57              |
| 40:RU:96:ALA:O     | 40:RU:100:VAL:HG23 | 2.05                     | 0.57              |
| 43:RX:36:LYS:HE3   | 43:RX:54:VAL:O     | 2.04                     | 0.57              |
| 1:XA:452:A:H62     | 1:XA:480:U:H3      | 1.53                     | 0.57              |
| 1:XA:792:A:H4'     | 1:XA:793:U:O5'     | 2.04                     | 0.57              |
| 7:XG:16:LEU:CD1    | 9:XI:45:ALA:HB2    | 2.34                     | 0.57              |
| 18:XR:25:THR:C     | 18:XR:26:LEU:HD23  | 2.29                     | 0.57              |
| 25:YA:631:A:OP2    | 54:Y8:46:ARG:NH2   | 2.34                     | 0.57              |
| 25:YA:1006:C:H1'   | 33:YN:106:MET:HE2  | 1.86                     | 0.57              |
| 25:YA:1957:C:H2'   | 25:YA:1958:C:H6    | 1.69                     | 0.57              |
| 25:YA:2364:C:OP1   | 46:Y0:55:ARG:NH1   | 2.37                     | 0.57              |
| 28:YE:102:VAL:HG13 | 28:YE:172:VAL:CG2  | 2.34                     | 0.57              |
| 30:YG:125:PHE:C    | 30:YG:127:GLY:H    | 2.12                     | 0.57              |
| 31:YH:2:SER:O      | 31:YH:3:ARG:C      | 2.47                     | 0.57              |
| 49:Y3:31:LEU:O     | 49:Y3:32:GLN:HB2   | 2.04                     | 0.57              |
| 50:Y4:42:PHE:CG    | 50:Y4:43:TYR:N     | 2.72                     | 0.57              |
| 54:Y8:46:ARG:O     | 54:Y8:47:LYS:HB3   | 2.03                     | 0.57              |
| 1:QA:1112:C:H1'    | 3:QC:179:ARG:HH11  | 1.69                     | 0.57              |
| 2:QB:106:LYS:O     | 2:QB:110:GLN:HG3   | 2.05                     | 0.57              |
| 25:RA:2469:A:H5''  | 25:RA:2470:G:C8    | 2.40                     | 0.57              |
| 28:RE:41:LYS:HA    | 28:RE:41:LYS:HE2   | 1.86                     | 0.57              |
| 28:RE:102:VAL:HG13 | 28:RE:172:VAL:CG2  | 2.34                     | 0.57              |
| 33:RN:63:THR:HG22  | 33:RN:66:LYS:NZ    | 2.20                     | 0.57              |
| 33:RN:112:LEU:C    | 33:RN:112:LEU:HD23 | 2.30                     | 0.57              |
| 34:RO:96:THR:O     | 34:RO:97:ARG:HB3   | 2.03                     | 0.57              |
| 47:R1:70:VAL:O     | 47:R1:74:VAL:HG23  | 2.05                     | 0.57              |
| 49:R3:31:LEU:O     | 49:R3:32:GLN:HB2   | 2.04                     | 0.57              |
| 52:R6:48:VAL:HG13  | 52:R6:49:HIS:N     | 2.20                     | 0.57              |
| 1:XA:1229:A:O2'    | 22:XV:30:G:OP1     | 2.16                     | 0.57              |
| 1:XA:1296:C:H3'    | 1:XA:1297:C:H6     | 1.70                     | 0.57              |
| 1:XA:1450:U:O2'    | 1:XA:1451:A:N7     | 2.37                     | 0.57              |
| 10:XJ:3:LYS:O      | 10:XJ:100:THR:HG22 | 2.04                     | 0.57              |
| 10:XJ:64:GLU:OE2   | 10:XJ:66:ARG:HD2   | 2.05                     | 0.57              |
| 27:YD:25:THR:HG21  | 27:YD:82:ILE:H     | 1.70                     | 0.57              |
| 27:YD:34:VAL:O     | 27:YD:34:VAL:CG1   | 2.51                     | 0.57              |
| 27:YD:36:PRO:HB2   | 27:YD:61:LEU:HG    | 1.87                     | 0.57              |
| 33:YN:63:THR:HG22  | 33:YN:66:LYS:NZ    | 2.20                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:YN:114:ARG:C   | 33:YN:116:LEU:H   | 2.13                     | 0.57              |
| 37:YR:45:ARG:HA   | 37:YR:95:THR:HG21 | 1.87                     | 0.57              |
| 42:YW:20:VAL:C    | 42:YW:22:ASP:N    | 2.60                     | 0.57              |
| 53:Y7:48:LYS:HG2  | 53:Y7:49:ARG:N    | 2.19                     | 0.57              |
| 1:QA:503:C:OP2    | 12:QL:116:SER:HB3 | 2.04                     | 0.57              |
| 1:QA:522:C:H41    | 12:QL:53:ARG:NH2  | 2.01                     | 0.57              |
| 1:QA:1152:A:H5'   | 10:QJ:13:HIS:CD2  | 2.39                     | 0.57              |
| 1:QA:1450:U:O2'   | 1:QA:1451:A:N7    | 2.37                     | 0.57              |
| 2:QB:30:ARG:HH21  | 2:QB:194:PRO:CG   | 2.17                     | 0.57              |
| 3:QC:59:ARG:NH2   | 3:QC:97:LYS:HE3   | 2.20                     | 0.57              |
| 4:QD:119:GLN:HG3  | 4:QD:123:HIS:CD2  | 2.40                     | 0.57              |
| 5:QE:140:ARG:HB2  | 5:QE:140:ARG:HH11 | 1.69                     | 0.57              |
| 7:QG:113:GLU:HB2  | 7:QG:119:ARG:CG   | 2.35                     | 0.57              |
| 11:QK:29:ILE:HG13 | 11:QK:43:SER:O    | 2.04                     | 0.57              |
| 13:QM:69:GLU:O    | 13:QM:71:ARG:N    | 2.38                     | 0.57              |
| 25:RA:1885:A:H5'  | 25:RA:1886:C:OP2  | 2.05                     | 0.57              |
| 25:RA:2311:A:H1'  | 30:RG:82:LEU:HD11 | 1.86                     | 0.57              |
| 33:RN:14:VAL:HG12 | 33:RN:15:LEU:H    | 1.69                     | 0.57              |
| 40:RU:68:ALA:O    | 40:RU:71:GLN:HB2  | 2.04                     | 0.57              |
| 47:R1:89:GLU:O    | 47:R1:93:GLU:HB2  | 2.05                     | 0.57              |
| 6:XF:99:ALA:O     | 6:XF:100:ASN:HB2  | 2.04                     | 0.57              |
| 14:XN:29:ARG:HH11 | 14:XN:29:ARG:HG3  | 1.70                     | 0.57              |
| 17:XQ:32:TYR:O    | 17:XQ:34:LYS:N    | 2.37                     | 0.57              |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HB1  | 1.86                     | 0.57              |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2 | 2.39                     | 0.57              |
| 29:YF:32:LEU:HD13 | 29:YF:105:VAL:CG1 | 2.33                     | 0.57              |
| 33:YN:7:LYS:HG2   | 33:YN:8:GLN:N     | 2.20                     | 0.57              |
| 34:YO:96:THR:O    | 34:YO:97:ARG:HB3  | 2.04                     | 0.57              |
| 44:YY:21:LYS:HG3  | 44:YY:22:GLY:H    | 1.69                     | 0.57              |
| 47:Y1:70:VAL:O    | 47:Y1:74:VAL:HG23 | 2.04                     | 0.57              |
| 50:Y4:39:CYS:O    | 50:Y4:40:HIS:HB2  | 2.03                     | 0.57              |
| 3:QC:59:ARG:HH12  | 3:QC:97:LYS:HE3   | 1.70                     | 0.57              |
| 8:QH:119:LEU:HD12 | 8:QH:124:ALA:HA   | 1.87                     | 0.57              |
| 10:QJ:74:ILE:HD13 | 10:QJ:74:ILE:N    | 2.16                     | 0.57              |
| 10:QJ:94:VAL:HG12 | 10:QJ:95:GLU:N    | 2.19                     | 0.57              |
| 15:QO:53:HIS:CE1  | 15:QO:57:LEU:HD11 | 2.40                     | 0.57              |
| 17:QQ:6:LEU:O     | 17:QQ:58:GLU:HA   | 2.05                     | 0.57              |
| 25:RA:78:A:H2'    | 25:RA:79:G:C8     | 2.40                     | 0.57              |
| 25:RA:1043:C:N3   | 25:RA:1112:G:N2   | 2.43                     | 0.57              |
| 25:RA:1818:U:O2'  | 27:RD:154:LYS:O   | 2.18                     | 0.57              |
| 25:RA:2451:A:N1   | 56:Z6:76:PPU:HE2  | 2.19                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:63:LEU:HD12 | 28:RE:65:GLY:H     | 1.69                     | 0.57              |
| 33:RN:82:LEU:HD12 | 33:RN:83:LYS:H     | 1.70                     | 0.57              |
| 33:RN:114:ARG:C   | 33:RN:116:LEU:H    | 2.13                     | 0.57              |
| 38:RS:72:ALA:O    | 38:RS:76:LYS:HG3   | 2.04                     | 0.57              |
| 44:RY:89:PHE:O    | 44:RY:90:LEU:HD13  | 2.05                     | 0.57              |
| 48:R2:31:GLU:O    | 48:R2:35:LEU:HG    | 2.05                     | 0.57              |
| 55:R9:1:MET:HB3   | 55:R9:4:ARG:CZ     | 2.35                     | 0.57              |
| 2:XB:30:ARG:HH21  | 2:XB:194:PRO:CG    | 2.18                     | 0.57              |
| 2:XB:187:LEU:CD1  | 2:XB:205:ASP:HA    | 2.34                     | 0.57              |
| 3:XC:11:ARG:HH21  | 3:XC:180:ALA:HB3   | 1.70                     | 0.57              |
| 4:XD:50:ARG:O     | 4:XD:50:ARG:HD2    | 2.05                     | 0.57              |
| 13:XM:82:MET:O    | 13:XM:84:ILE:N     | 2.38                     | 0.57              |
| 14:XN:13:THR:N    | 14:XN:14:PRO:CD    | 2.68                     | 0.57              |
| 16:XP:7:ALA:O     | 16:XP:9:PHE:CD2    | 2.58                     | 0.57              |
| 16:XP:21:VAL:HG22 | 16:XP:34:GLU:O     | 2.04                     | 0.57              |
| 25:YA:1500:G:O2'  | 27:YD:100:GLY:O    | 2.16                     | 0.57              |
| 25:YA:1939:U:OP1  | 25:YA:2604:U:O2'   | 2.15                     | 0.57              |
| 29:YF:118:ALA:O   | 29:YF:121:GLY:N    | 2.33                     | 0.57              |
| 1:QA:347:G:O2'    | 1:QA:348:G:H5''    | 2.04                     | 0.56              |
| 3:QC:7:PRO:O      | 3:QC:11:ARG:HG2    | 2.05                     | 0.56              |
| 3:QC:76:VAL:HG21  | 3:QC:103:VAL:CG1   | 2.34                     | 0.56              |
| 7:QG:18:TYR:HD2   | 7:QG:59:LEU:HD22   | 1.70                     | 0.56              |
| 7:QG:121:ALA:O    | 7:QG:125:MET:N     | 2.37                     | 0.56              |
| 8:QH:84:ARG:NH1   | 8:QH:86:ILE:HD13   | 2.11                     | 0.56              |
| 9:QI:17:VAL:CG1   | 9:QI:81:ILE:HD13   | 2.35                     | 0.56              |
| 11:QK:69:ALA:HB1  | 11:QK:103:LEU:CD2  | 2.35                     | 0.56              |
| 12:QL:45:PRO:HD3  | 12:QL:51:ALA:O     | 2.04                     | 0.56              |
| 14:QN:8:GLU:C     | 14:QN:10:ALA:H     | 2.13                     | 0.56              |
| 16:QP:14:ASN:N    | 16:QP:15:PRO:CD    | 2.67                     | 0.56              |
| 25:RA:2394:C:OP1  | 35:RP:63:PRO:HD2   | 2.05                     | 0.56              |
| 25:RA:2698:U:H2'  | 25:RA:2699:C:C6    | 2.39                     | 0.56              |
| 25:RA:2712:U:HO2' | 25:RA:2712(A):A:H8 | 1.53                     | 0.56              |
| 27:RD:35:LYS:CE   | 27:RD:104:TYR:HB2  | 2.35                     | 0.56              |
| 31:RH:3:ARG:HA    | 31:RH:3:ARG:HE     | 1.69                     | 0.56              |
| 33:RN:112:LEU:O   | 33:RN:114:ARG:O    | 2.23                     | 0.56              |
| 37:RR:56:LYS:C    | 37:RR:58:GLY:N     | 2.62                     | 0.56              |
| 50:R4:50:VAL:O    | 50:R4:51:ASP:C     | 2.48                     | 0.56              |
| 52:R6:11:LEU:HD23 | 52:R6:26:ASN:HB3   | 1.87                     | 0.56              |
| 53:R7:19:ARG:HH11 | 53:R7:19:ARG:HG2   | 1.70                     | 0.56              |
| 53:R7:38:GLY:O    | 53:R7:39:ARG:C     | 2.48                     | 0.56              |
| 2:XB:60:ASP:HB3   | 2:XB:64:ARG:CZ     | 2.34                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:XM:49:THR:HB   | 13:XM:52:GLU:HG3  | 1.86                     | 0.56              |
| 13:XM:69:GLU:O    | 13:XM:71:ARG:N    | 2.38                     | 0.56              |
| 25:YA:389:G:H1    | 35:YP:71:VAL:HG12 | 1.69                     | 0.56              |
| 25:YA:2271:G:OP1  | 46:Y0:18:ALA:HB1  | 2.05                     | 0.56              |
| 30:YG:60:LEU:O    | 30:YG:64:THR:HG22 | 2.05                     | 0.56              |
| 38:YS:67:ARG:CB   | 38:YS:67:ARG:HH11 | 2.18                     | 0.56              |
| 40:YU:83:LEU:HD12 | 40:YU:113:ALA:HB2 | 1.86                     | 0.56              |
| 44:YY:97:ARG:HG2  | 44:YY:97:ARG:O    | 2.05                     | 0.56              |
| 1:QA:895:G:H1     | 1:QA:904:C:H42    | 1.53                     | 0.56              |
| 2:QB:60:ASP:HB3   | 2:QB:64:ARG:CZ    | 2.35                     | 0.56              |
| 11:QK:21:ILE:HD12 | 11:QK:21:ILE:N    | 2.19                     | 0.56              |
| 13:QM:4:ILE:HG22  | 13:QM:5:ALA:N     | 2.19                     | 0.56              |
| 25:RA:299:A:H5'   | 44:RY:84:ARG:HH21 | 1.70                     | 0.56              |
| 25:RA:2232:U:P    | 47:R1:40:ARG:HH12 | 2.28                     | 0.56              |
| 25:RA:2343:C:HO2' | 25:RA:2373:G:HO2' | 1.53                     | 0.56              |
| 26:RB:55:U:H5''   | 30:RG:28:VAL:HG21 | 1.87                     | 0.56              |
| 28:RE:152:LYS:HG2 | 33:RN:78:TYR:CE1  | 2.40                     | 0.56              |
| 29:RF:24:LEU:HB3  | 29:RF:115:ALA:HB2 | 1.87                     | 0.56              |
| 35:RP:13:ASN:O    | 35:RP:14:LYS:C    | 2.49                     | 0.56              |
| 35:RP:31:ALA:O    | 35:RP:32:THR:HG23 | 2.05                     | 0.56              |
| 37:RR:70:LEU:HD13 | 37:RR:75:LEU:HD11 | 1.88                     | 0.56              |
| 41:RV:38:LEU:HD23 | 41:RV:39:LEU:N    | 2.19                     | 0.56              |
| 49:R3:4:LEU:O     | 49:R3:36:VAL:HA   | 2.04                     | 0.56              |
| 53:R7:13:ALA:O    | 53:R7:17:GLY:HA3  | 2.05                     | 0.56              |
| 1:XA:1086:U:H3    | 1:XA:1099:G:H22   | 1.52                     | 0.56              |
| 2:XB:80:ILE:CG2   | 2:XB:212:GLN:HA   | 2.35                     | 0.56              |
| 4:XD:76:ARG:HD2   | 4:XD:207:TYR:HE2  | 1.66                     | 0.56              |
| 4:XD:100:ARG:HH22 | 4:XD:137:SER:HB3  | 1.70                     | 0.56              |
| 5:XE:78:HIS:CE1   | 5:XE:143:ARG:H    | 2.20                     | 0.56              |
| 7:XG:42:ILE:O     | 7:XG:117:ALA:HB2  | 2.05                     | 0.56              |
| 8:XH:49:GLU:HG3   | 8:XH:51:VAL:CG1   | 2.35                     | 0.56              |
| 19:XS:9:VAL:O     | 19:XS:9:VAL:HG23  | 2.04                     | 0.56              |
| 25:YA:709:U:H2'   | 25:YA:710:G:H8    | 1.70                     | 0.56              |
| 25:YA:1266:G:O5'  | 42:YW:15:ARG:NH2  | 2.37                     | 0.56              |
| 25:YA:1434:A:H61  | 25:YA:1558:A:N6   | 2.03                     | 0.56              |
| 25:YA:2168:G:N2   | 25:YA:2170:A:N7   | 2.53                     | 0.56              |
| 30:YG:39:ILE:CG2  | 30:YG:155:MET:HG3 | 2.35                     | 0.56              |
| 31:YH:77:LYS:HZ3  | 31:YH:77:LYS:CB   | 2.11                     | 0.56              |
| 31:YH:84:SER:O    | 31:YH:133:VAL:O   | 2.22                     | 0.56              |
| 35:YP:59:LEU:HA   | 35:YP:61:ARG:CZ   | 2.35                     | 0.56              |
| 36:YQ:37:LEU:HD21 | 36:YQ:130:LYS:HE3 | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:134:GLU:O    | 39:YT:135:ALA:HB3  | 2.05                     | 0.56              |
| 48:Y2:17:SER:HB2   | 48:Y2:18:PRO:HA    | 1.86                     | 0.56              |
| 49:Y3:7:LYS:NZ     | 49:Y3:32:GLN:HE21  | 2.03                     | 0.56              |
| 52:Y6:14:THR:O     | 52:Y6:49:HIS:HA    | 2.06                     | 0.56              |
| 53:Y7:38:GLY:O     | 53:Y7:39:ARG:C     | 2.48                     | 0.56              |
| 1:QA:321:A:N6      | 1:QA:329:A:OP2     | 2.38                     | 0.56              |
| 1:QA:1199:U:H4'    | 10:QJ:54:PHE:CZ    | 2.40                     | 0.56              |
| 2:QB:77:ALA:CB     | 2:QB:211:ILE:HG21  | 2.35                     | 0.56              |
| 3:QC:188:LEU:O     | 3:QC:189:ALA:HB2   | 2.05                     | 0.56              |
| 9:QI:13:ALA:HB2    | 9:QI:67:GLY:C      | 2.28                     | 0.56              |
| 12:QL:10:LEU:HB3   | 17:QQ:32:TYR:CZ    | 2.41                     | 0.56              |
| 12:QL:58:VAL:O     | 12:QL:65:GLU:HA    | 2.06                     | 0.56              |
| 13:QM:84:ILE:CG2   | 13:QM:85:GLY:N     | 2.68                     | 0.56              |
| 14:QN:25:VAL:N     | 14:QN:38:GLY:O     | 2.38                     | 0.56              |
| 16:QP:7:ALA:O      | 16:QP:9:PHE:CD2    | 2.59                     | 0.56              |
| 19:QS:40:ILE:HG12  | 19:QS:41:VAL:N     | 2.21                     | 0.56              |
| 20:QT:53:LEU:HA    | 20:QT:56:MET:HB3   | 1.87                     | 0.56              |
| 20:QT:82:SER:O     | 20:QT:86:ARG:HB2   | 2.05                     | 0.56              |
| 21:QU:7:ARG:O      | 21:QU:8:THR:HG23   | 2.05                     | 0.56              |
| 25:RA:76:C:O2'     | 48:R2:62:THR:HG21  | 2.05                     | 0.56              |
| 25:RA:84:A:N1      | 25:RA:98:G:O2'     | 2.30                     | 0.56              |
| 25:RA:227:A:OP1    | 35:RP:76:LYS:HE3   | 2.05                     | 0.56              |
| 25:RA:483:A:H4'    | 44:RY:49:VAL:HG13  | 1.86                     | 0.56              |
| 25:RA:483:A:H3'    | 25:RA:484:C:H6     | 1.70                     | 0.56              |
| 25:RA:1006:C:H1'   | 33:RN:106:MET:HE2  | 1.88                     | 0.56              |
| 25:RA:1264:G:H3'   | 25:RA:1265:A:H5''  | 1.87                     | 0.56              |
| 25:RA:1638:C:O2    | 25:RA:2698:U:O2'   | 2.23                     | 0.56              |
| 25:RA:2445:G:OP1   | 29:RF:74:ARG:NH2   | 2.37                     | 0.56              |
| 27:RD:236:GLY:O    | 27:RD:237:GLU:OE1  | 2.23                     | 0.56              |
| 28:RE:78:LEU:HD23  | 28:RE:79:ARG:HD2   | 1.86                     | 0.56              |
| 28:RE:183:LEU:HD12 | 28:RE:183:LEU:N    | 2.20                     | 0.56              |
| 29:RF:46:ARG:HG2   | 29:RF:46:ARG:NH1   | 2.00                     | 0.56              |
| 29:RF:198:ALA:CA   | 29:RF:201:VAL:HG12 | 2.35                     | 0.56              |
| 30:RG:97:ASP:H     | 30:RG:100:TRP:CD1  | 2.18                     | 0.56              |
| 31:RH:2:SER:O      | 31:RH:3:ARG:C      | 2.47                     | 0.56              |
| 33:RN:56:ASN:N     | 33:RN:125:GLY:O    | 2.35                     | 0.56              |
| 38:RS:5:THR:HG23   | 38:RS:8:GLU:OE2    | 2.05                     | 0.56              |
| 38:RS:32:LEU:O     | 38:RS:62:LYS:HE2   | 2.06                     | 0.56              |
| 40:RU:39:LEU:O     | 40:RU:40:PHE:C     | 2.48                     | 0.56              |
| 44:RY:97:ARG:O     | 44:RY:97:ARG:HG2   | 2.05                     | 0.56              |
| 48:R2:51:ARG:HA    | 48:R2:54:LYS:HB2   | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:R5:55:ARG:HD3   | 51:R5:56:LYS:N     | 2.21                     | 0.56              |
| 52:R6:14:THR:O     | 52:R6:49:HIS:HA    | 2.06                     | 0.56              |
| 52:R6:42:TRP:N     | 52:R6:42:TRP:CD1   | 2.73                     | 0.56              |
| 54:R8:52:LYS:H     | 54:R8:53:PRO:HD2   | 1.66                     | 0.56              |
| 1:XA:581:G:N2      | 1:XA:760:G:N7      | 2.54                     | 0.56              |
| 1:XA:1132:C:H2'    | 1:XA:1133:G:C8     | 2.40                     | 0.56              |
| 2:XB:55:PHE:HA     | 2:XB:58:ILE:HB     | 1.88                     | 0.56              |
| 2:XB:102:LEU:HB3   | 2:XB:180:LEU:CD1   | 2.36                     | 0.56              |
| 3:XC:57:ILE:HG23   | 3:XC:64:VAL:HG13   | 1.86                     | 0.56              |
| 3:XC:59:ARG:HH12   | 3:XC:97:LYS:HE3    | 1.70                     | 0.56              |
| 3:XC:105:GLU:HG2   | 3:XC:106:VAL:N     | 2.18                     | 0.56              |
| 6:XF:92:LYS:HB2    | 6:XF:92:LYS:HZ2    | 1.70                     | 0.56              |
| 7:XG:18:TYR:HD2    | 7:XG:59:LEU:HD22   | 1.70                     | 0.56              |
| 9:XI:10:ARG:CD     | 9:XI:105:ASP:HB2   | 2.35                     | 0.56              |
| 9:XI:33:PHE:CE2    | 9:XI:47:LEU:HD21   | 2.40                     | 0.56              |
| 11:XK:34:ASP:N     | 11:XK:40:ILE:HD11  | 2.20                     | 0.56              |
| 16:XP:4:ILE:HA     | 16:XP:20:VAL:O     | 2.05                     | 0.56              |
| 21:XU:7:ARG:O      | 21:XU:8:THR:HG23   | 2.05                     | 0.56              |
| 23:XY:41:A:O2'     | 23:XY:42:G:OP1     | 2.21                     | 0.56              |
| 25:YA:83:G:HO2'    | 25:YA:84:A:H8      | 1.49                     | 0.56              |
| 25:YA:1012:U:O2'   | 25:YA:1013:C:OP2   | 2.20                     | 0.56              |
| 25:YA:2832:U:H4'   | 25:YA:2833:G:C5'   | 2.35                     | 0.56              |
| 27:YD:69:ARG:HD3   | 27:YD:105:ILE:HD11 | 1.87                     | 0.56              |
| 27:YD:183:ARG:HD2  | 27:YD:270:ILE:HG12 | 1.88                     | 0.56              |
| 30:YG:34:LEU:HD13  | 30:YG:34:LEU:C     | 2.30                     | 0.56              |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CG   | 2.34                     | 0.56              |
| 33:YN:82:LEU:HD12  | 33:YN:83:LYS:H     | 1.70                     | 0.56              |
| 34:YO:3:GLN:CB     | 34:YO:4:PRO:HD2    | 2.35                     | 0.56              |
| 38:YS:103:GLU:O    | 38:YS:106:ARG:CG   | 2.52                     | 0.56              |
| 39:YT:26:ASP:CB    | 39:YT:91:ARG:HA    | 2.36                     | 0.56              |
| 40:YU:68:ALA:O     | 40:YU:71:GLN:HB2   | 2.04                     | 0.56              |
| 41:YV:76:LYS:O     | 41:YV:79:VAL:HG12  | 2.05                     | 0.56              |
| 43:YX:35:THR:HG22  | 43:YX:38:GLU:OE1   | 2.05                     | 0.56              |
| 47:Y1:89:GLU:O     | 47:Y1:93:GLU:HB2   | 2.05                     | 0.56              |
| 48:Y2:31:GLU:O     | 48:Y2:35:LEU:HG    | 2.05                     | 0.56              |
| 50:Y4:15:ILE:HG22  | 50:Y4:20:ASN:HA    | 1.86                     | 0.56              |
| 50:Y4:27:THR:O     | 50:Y4:28:LYS:HB3   | 2.04                     | 0.56              |
| 53:Y7:12:ARG:NH2   | 53:Y7:44:PRO:HB3   | 2.21                     | 0.56              |
| 55:Y9:2:LYS:HD2    | 55:Y9:33:LYS:O     | 2.05                     | 0.56              |
| 55:Y9:25:VAL:HB    | 55:Y9:34:GLN:HB2   | 1.86                     | 0.56              |
| 1:QA:584:G:H2'     | 1:QA:585:G:C8      | 2.40                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:QC:114:PRO:O     | 3:QC:118:GLN:HG3  | 2.06                     | 0.56              |
| 5:QE:82:VAL:CG1    | 5:QE:83:GLU:N     | 2.68                     | 0.56              |
| 12:QL:18:VAL:O     | 12:QL:19:ARG:HB2  | 2.04                     | 0.56              |
| 13:QM:73:GLU:O     | 13:QM:77:ASN:N    | 2.33                     | 0.56              |
| 17:QQ:50:LYS:HG3   | 17:QQ:51:TYR:CE1  | 2.40                     | 0.56              |
| 25:RA:1794:U:H2'   | 25:RA:1795:C:C6   | 2.41                     | 0.56              |
| 25:RA:2777:G:OP2   | 25:RA:2781:A:O2'  | 2.20                     | 0.56              |
| 28:RE:37:ARG:NE    | 28:RE:37:ARG:N    | 2.54                     | 0.56              |
| 29:RF:32:LEU:HD13  | 29:RF:105:VAL:CG1 | 2.33                     | 0.56              |
| 30:RG:41:GLN:HB3   | 30:RG:43:LEU:HD13 | 1.87                     | 0.56              |
| 31:RH:77:LYS:HZ3   | 31:RH:77:LYS:CB   | 2.03                     | 0.56              |
| 34:RO:19:ILE:HD13  | 34:RO:19:ILE:O    | 2.06                     | 0.56              |
| 35:RP:31:ALA:C     | 35:RP:32:THR:HG23 | 2.31                     | 0.56              |
| 35:RP:65:ARG:HH21  | 54:R8:15:LYS:CB   | 2.17                     | 0.56              |
| 47:R1:53:VAL:HG12  | 47:R1:54:ALA:N    | 2.21                     | 0.56              |
| 50:R4:48:ARG:HH12  | 50:R4:52:THR:HG22 | 1.70                     | 0.56              |
| 1:XA:1320:C:H42    | 19:XS:36:ARG:HG3  | 1.69                     | 0.56              |
| 4:XD:42:GLN:HG2    | 4:XD:42:GLN:O     | 2.05                     | 0.56              |
| 6:XF:91:VAL:CG1    | 18:XR:72:ARG:HH12 | 2.18                     | 0.56              |
| 7:XG:148:ASN:N     | 7:XG:148:ASN:ND2  | 2.46                     | 0.56              |
| 8:XH:38:ILE:HD12   | 8:XH:118:VAL:HG12 | 1.87                     | 0.56              |
| 11:XK:32:ILE:O     | 11:XK:40:ILE:HG12 | 2.04                     | 0.56              |
| 19:XS:5:LEU:HD21   | 50:Y4:66:SER:CB   | 2.35                     | 0.56              |
| 25:YA:1454:U:H5'   | 37:YR:63:ARG:NE   | 2.19                     | 0.56              |
| 25:YA:2295:C:OP1   | 38:YS:10:ARG:HD2  | 2.06                     | 0.56              |
| 25:YA:2311:A:C1'   | 30:YG:82:LEU:HD11 | 2.35                     | 0.56              |
| 27:YD:2:ALA:O      | 27:YD:3:VAL:HB    | 2.06                     | 0.56              |
| 28:YE:37:ARG:NE    | 28:YE:37:ARG:N    | 2.53                     | 0.56              |
| 28:YE:74:PRO:HG2   | 28:YE:77:ILE:HG23 | 1.87                     | 0.56              |
| 33:YN:56:ASN:N     | 33:YN:125:GLY:O   | 2.35                     | 0.56              |
| 33:YN:112:LEU:HD23 | 33:YN:112:LEU:C   | 2.30                     | 0.56              |
| 36:YQ:79:LEU:O     | 36:YQ:79:LEU:CG   | 2.52                     | 0.56              |
| 4:QD:42:GLN:HG2    | 4:QD:42:GLN:O     | 2.05                     | 0.56              |
| 9:QI:10:ARG:CD     | 9:QI:105:ASP:HB2  | 2.35                     | 0.56              |
| 10:QJ:24:VAL:HG21  | 10:QJ:37:PRO:HG3  | 1.86                     | 0.56              |
| 17:QQ:48:GLU:O     | 17:QQ:49:GLU:C    | 2.48                     | 0.56              |
| 25:RA:1796:U:H2'   | 25:RA:1797:C:H6   | 1.70                     | 0.56              |
| 25:RA:2636:U:OP1   | 28:RE:79:ARG:HA   | 2.06                     | 0.56              |
| 26:RB:45:A:H1'     | 30:RG:95:ARG:HH22 | 1.71                     | 0.56              |
| 28:RE:32:PRO:O     | 28:RE:34:VAL:HG13 | 2.06                     | 0.56              |
| 28:RE:117:MET:O    | 28:RE:117:MET:HG3 | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:RG:34:LEU:HD13 | 30:RG:34:LEU:C    | 2.30                     | 0.56              |
| 30:RG:34:LEU:HD11 | 30:RG:99:MET:HE2  | 1.88                     | 0.56              |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:HZ1  | 1.67                     | 0.56              |
| 35:RP:14:LYS:O    | 35:RP:16:ARG:N    | 2.39                     | 0.56              |
| 36:RQ:79:LEU:O    | 36:RQ:79:LEU:CG   | 2.52                     | 0.56              |
| 39:RT:26:ASP:CB   | 39:RT:91:ARG:HA   | 2.36                     | 0.56              |
| 50:R4:48:ARG:O    | 50:R4:50:VAL:N    | 2.38                     | 0.56              |
| 55:R9:2:LYS:HD2   | 55:R9:33:LYS:O    | 2.04                     | 0.56              |
| 3:XC:7:PRO:O      | 3:XC:11:ARG:HG2   | 2.05                     | 0.56              |
| 3:XC:90:GLU:O     | 3:XC:94:LEU:HG    | 2.05                     | 0.56              |
| 8:XH:82:HIS:HD2   | 8:XH:83:ILE:N     | 2.03                     | 0.56              |
| 10:XJ:35:SER:O    | 10:XJ:72:VAL:HG13 | 2.05                     | 0.56              |
| 10:XJ:94:VAL:HG12 | 10:XJ:95:GLU:N    | 2.19                     | 0.56              |
| 11:XK:69:ALA:HB1  | 11:XK:103:LEU:CD2 | 2.35                     | 0.56              |
| 13:XM:84:ILE:CG2  | 13:XM:85:GLY:N    | 2.68                     | 0.56              |
| 15:XO:53:HIS:CE1  | 15:XO:57:LEU:HD11 | 2.40                     | 0.56              |
| 19:XS:17:GLU:HA   | 19:XS:20:LEU:HD12 | 1.86                     | 0.56              |
| 20:XT:82:SER:O    | 20:XT:86:ARG:HB2  | 2.05                     | 0.56              |
| 21:XU:6:ARG:HH21  | 21:XU:15:ARG:HE   | 1.53                     | 0.56              |
| 25:YA:2344:U:C2   | 52:Y6:37:ARG:HD3  | 2.40                     | 0.56              |
| 28:YE:32:PRO:O    | 28:YE:34:VAL:HG13 | 2.06                     | 0.56              |
| 28:YE:77:ILE:O    | 28:YE:78:LEU:C    | 2.48                     | 0.56              |
| 31:YH:6:ARG:C     | 31:YH:8:PRO:HD2   | 2.30                     | 0.56              |
| 35:YP:59:LEU:O    | 35:YP:59:LEU:HD23 | 2.06                     | 0.56              |
| 38:YS:32:LEU:O    | 38:YS:62:LYS:HE2  | 2.05                     | 0.56              |
| 40:YU:104:GLN:OE1 | 40:YU:104:GLN:N   | 2.35                     | 0.56              |
| 44:YY:75:ILE:C    | 44:YY:75:ILE:HD13 | 2.31                     | 0.56              |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CG   | 2.36                     | 0.56              |
| 54:Y8:50:LEU:HD12 | 54:Y8:51:ALA:H    | 1.70                     | 0.56              |
| 1:QA:411:A:C4     | 1:QA:413:G:H1'    | 2.41                     | 0.56              |
| 3:QC:134:ILE:CD1  | 3:QC:153:VAL:HG21 | 2.35                     | 0.56              |
| 5:QE:99:GLY:O     | 5:QE:117:ASP:HA   | 2.06                     | 0.56              |
| 8:QH:7:ALA:HB2    | 8:QH:85:ARG:HD3   | 1.87                     | 0.56              |
| 8:QH:77:GLU:HG2   | 8:QH:78:GLN:H     | 1.71                     | 0.56              |
| 9:QI:9:ARG:HB2    | 9:QI:14:VAL:HG22  | 1.88                     | 0.56              |
| 12:QL:82:VAL:HG23 | 12:QL:106:ASP:OD2 | 2.04                     | 0.56              |
| 14:QN:15:LYS:O    | 14:QN:16:PHE:O    | 2.24                     | 0.56              |
| 16:QP:4:ILE:HA    | 16:QP:20:VAL:O    | 2.05                     | 0.56              |
| 25:RA:1287:A:N7   | 37:RR:107:ASP:HB2 | 2.19                     | 0.56              |
| 25:RA:2208:U:O2'  | 27:RD:151:LYS:HG2 | 2.05                     | 0.56              |
| 38:RS:5:THR:OG1   | 38:RS:7:TYR:HB3   | 2.06                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:RT:134:GLU:O    | 39:RT:135:ALA:HB3  | 2.05                     | 0.56              |
| 41:RV:27:ALA:O     | 41:RV:28:GLU:O     | 2.24                     | 0.56              |
| 41:RV:75:PHE:C     | 41:RV:75:PHE:CD1   | 2.83                     | 0.56              |
| 44:RY:75:ILE:C     | 44:RY:75:ILE:HD13  | 2.30                     | 0.56              |
| 44:RY:95:LYS:O     | 44:RY:95:LYS:HE3   | 2.05                     | 0.56              |
| 53:R7:12:ARG:NH2   | 53:R7:44:PRO:HB3   | 2.21                     | 0.56              |
| 1:XA:486:U:H2'     | 1:XA:487:A:H8      | 1.71                     | 0.56              |
| 1:XA:1305:G:H21    | 1:XA:1331:G:H2'    | 1.68                     | 0.56              |
| 2:XB:178:ARG:HD2   | 8:XH:71:GLY:C      | 2.29                     | 0.56              |
| 3:XC:180:ALA:O     | 3:XC:181:ASN:HB3   | 2.06                     | 0.56              |
| 3:XC:188:LEU:O     | 3:XC:189:ALA:HB2   | 2.05                     | 0.56              |
| 4:XD:110:PHE:CE2   | 4:XD:148:VAL:HG23  | 2.41                     | 0.56              |
| 4:XD:119:GLN:HG3   | 4:XD:123:HIS:CD2   | 2.40                     | 0.56              |
| 6:XF:97:PHE:O      | 18:XR:31:LEU:HD23  | 2.04                     | 0.56              |
| 8:XH:7:ALA:HB2     | 8:XH:85:ARG:HD3    | 1.87                     | 0.56              |
| 25:YA:1535:U:H5''  | 25:YA:1537:C:C4    | 2.40                     | 0.56              |
| 25:YA:1803:A:N1    | 25:YA:1822:G:O2'   | 2.33                     | 0.56              |
| 27:YD:35:LYS:CE    | 27:YD:104:TYR:HB2  | 2.35                     | 0.56              |
| 29:YF:155:LEU:CD1  | 29:YF:174:VAL:HG13 | 2.32                     | 0.56              |
| 35:YP:115:LEU:HD12 | 35:YP:116:GLY:N    | 2.21                     | 0.56              |
| 41:YV:75:PHE:C     | 41:YV:75:PHE:CD1   | 2.83                     | 0.56              |
| 47:Y1:76:ARG:HG2   | 47:Y1:76:ARG:NH1   | 2.20                     | 0.56              |
| 1:QA:664:G:H22     | 1:QA:741:G:H1      | 1.53                     | 0.56              |
| 1:QA:864:A:H5'     | 5:QE:86:ALA:HB2    | 1.88                     | 0.56              |
| 2:QB:7:VAL:HG22    | 2:QB:8:LYS:N       | 2.21                     | 0.56              |
| 3:QC:33:LEU:O      | 3:QC:37:GLN:HG2    | 2.04                     | 0.56              |
| 4:QD:110:PHE:CE2   | 4:QD:148:VAL:HG23  | 2.41                     | 0.56              |
| 5:QE:107:ARG:O     | 5:QE:108:ALA:C     | 2.49                     | 0.56              |
| 6:QF:33:TYR:HE2    | 6:QF:74:ASP:HB3    | 1.71                     | 0.56              |
| 6:QF:69:GLU:C      | 6:QF:71:ARG:H      | 2.13                     | 0.56              |
| 9:QI:33:PHE:CE2    | 9:QI:47:LEU:HD21   | 2.40                     | 0.56              |
| 15:QO:24:SER:O     | 15:QO:28:GLN:HG3   | 2.06                     | 0.56              |
| 19:QS:15:LEU:HD23  | 19:QS:15:LEU:N     | 2.20                     | 0.56              |
| 25:RA:137(A):G:H1' | 43:RX:41:ASN:ND2   | 2.20                     | 0.56              |
| 25:RA:336:C:H5''   | 44:RY:6:HIS:CD2    | 2.41                     | 0.56              |
| 27:RD:80:ALA:HB3   | 27:RD:94:LEU:HD13  | 1.88                     | 0.56              |
| 29:RF:9:ILE:HD11   | 29:RF:125:LEU:CG   | 2.36                     | 0.56              |
| 30:RG:120:LEU:HB3  | 30:RG:131:TYR:OH   | 2.05                     | 0.56              |
| 37:RR:84:ALA:HB3   | 37:RR:85:PRO:HD3   | 1.88                     | 0.56              |
| 41:RV:76:LYS:O     | 41:RV:79:VAL:HG12  | 2.05                     | 0.56              |
| 43:RX:35:THR:HG22  | 43:RX:38:GLU:OE1   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:RX:65:ARG:HD3  | 43:RX:65:ARG:H     | 1.70                     | 0.56              |
| 47:R1:92:LYS:C    | 47:R1:94:LEU:N     | 2.62                     | 0.56              |
| 50:R4:41:PRO:O    | 50:R4:42:PHE:CB    | 2.54                     | 0.56              |
| 54:R8:50:LEU:HD12 | 54:R8:51:ALA:H     | 1.70                     | 0.56              |
| 1:XA:921:U:O2'    | 5:XE:19:MET:O      | 2.21                     | 0.56              |
| 2:XB:169:LYS:HD3  | 2:XB:169:LYS:O     | 2.05                     | 0.56              |
| 2:XB:178:ARG:HD2  | 8:XH:71:GLY:CA     | 2.35                     | 0.56              |
| 3:XC:114:PRO:O    | 3:XC:118:GLN:HG3   | 2.05                     | 0.56              |
| 4:XD:25:ARG:NH1   | 4:XD:30:LYS:HG3    | 2.20                     | 0.56              |
| 5:XE:82:VAL:CG1   | 5:XE:83:GLU:N      | 2.68                     | 0.56              |
| 7:XG:62:PHE:O     | 7:XG:66:VAL:HG23   | 2.06                     | 0.56              |
| 11:XK:21:ILE:HG13 | 11:XK:30:VAL:HG12  | 1.86                     | 0.56              |
| 13:XM:56:LEU:HD13 | 13:XM:60:VAL:HG23  | 1.86                     | 0.56              |
| 13:XM:89:GLY:O    | 13:XM:92:HIS:HB2   | 2.06                     | 0.56              |
| 18:XR:85:LEU:HD23 | 18:XR:88:LYS:HD2   | 1.86                     | 0.56              |
| 25:YA:869:G:H1    | 25:YA:908:C:H42    | 1.52                     | 0.56              |
| 29:YF:197:ASP:O   | 29:YF:199:TRP:N    | 2.38                     | 0.56              |
| 33:YN:112:LEU:O   | 33:YN:114:ARG:O    | 2.23                     | 0.56              |
| 50:Y4:48:ARG:O    | 50:Y4:50:VAL:N     | 2.38                     | 0.56              |
| 52:Y6:6:ARG:O     | 52:Y6:8:LYS:HD2    | 2.05                     | 0.56              |
| 53:Y7:13:ALA:O    | 53:Y7:17:GLY:HA3   | 2.05                     | 0.56              |
| 3:QC:6:HIS:CD2    | 3:QC:7:PRO:HD2     | 2.41                     | 0.56              |
| 5:QE:140:ARG:HH11 | 5:QE:140:ARG:CB    | 2.18                     | 0.56              |
| 8:QH:38:ILE:HD12  | 8:QH:118:VAL:HG12  | 1.87                     | 0.56              |
| 12:QL:83:VAL:HG22 | 12:QL:84:LEU:H     | 1.70                     | 0.56              |
| 20:QT:94:ALA:O    | 20:QT:95:ALA:CB    | 2.54                     | 0.56              |
| 25:RA:483:A:H3'   | 25:RA:484:C:C6     | 2.41                     | 0.56              |
| 25:RA:2680:C:H5'  | 28:RE:189:PRO:HA   | 1.86                     | 0.56              |
| 27:RD:94:LEU:HD22 | 27:RD:95:LEU:H     | 1.69                     | 0.56              |
| 27:RD:183:ARG:HD2 | 27:RD:270:ILE:HG12 | 1.88                     | 0.56              |
| 30:RG:60:LEU:O    | 30:RG:64:THR:HG22  | 2.05                     | 0.56              |
| 31:RH:153:LYS:CB  | 31:RH:154:PRO:CD   | 2.69                     | 0.56              |
| 36:RQ:12:GLN:OE1  | 36:RQ:72:LYS:HD2   | 2.06                     | 0.56              |
| 37:RR:1:MET:SD    | 37:RR:1:MET:N      | 2.75                     | 0.56              |
| 48:R2:50:ILE:CD1  | 48:R2:51:ARG:N     | 2.61                     | 0.56              |
| 49:R3:59:VAL:CG1  | 49:R3:60:GLU:N     | 2.69                     | 0.56              |
| 50:R4:37:SER:C    | 50:R4:39:CYS:N     | 2.62                     | 0.56              |
| 1:XA:537:G:H5''   | 12:XL:113:ARG:NH1  | 2.20                     | 0.56              |
| 1:XA:1132:C:H2'   | 1:XA:1133:G:H8     | 1.71                     | 0.56              |
| 1:XA:1346:A:H5'   | 9:XI:120:ARG:HH12  | 1.69                     | 0.56              |
| 4:XD:107:ARG:C    | 4:XD:109:GLY:H     | 2.14                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:XG:20:ASP:HB3    | 7:XG:23:VAL:HG23  | 1.88                     | 0.56              |
| 8:XH:77:GLU:HG2    | 8:XH:78:GLN:H     | 1.71                     | 0.56              |
| 9:XI:17:VAL:CG1    | 9:XI:81:ILE:HD13  | 2.35                     | 0.56              |
| 12:XL:111:LYS:O    | 12:XL:112:ASP:HB2 | 2.06                     | 0.56              |
| 14:XN:23:ARG:H     | 14:XN:33:VAL:HG11 | 1.71                     | 0.56              |
| 25:YA:207:A:H2'    | 25:YA:208:C:O4'   | 2.05                     | 0.56              |
| 25:YA:330:A:H2     | 25:YA:1210:A:H2'  | 1.70                     | 0.56              |
| 25:YA:1042:G:H1    | 25:YA:1113:U:H3   | 1.53                     | 0.56              |
| 25:YA:1717:G:H1    | 25:YA:1742:C:H42  | 1.53                     | 0.56              |
| 25:YA:2636:U:OP1   | 28:YE:79:ARG:HG3  | 2.05                     | 0.56              |
| 27:YD:259:THR:O    | 27:YD:260:ARG:C   | 2.49                     | 0.56              |
| 28:YE:183:LEU:HD12 | 28:YE:183:LEU:N   | 2.20                     | 0.56              |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:H   | 1.71                     | 0.56              |
| 30:YG:128:ARG:HG3  | 30:YG:128:ARG:NH2 | 2.17                     | 0.56              |
| 44:YY:94:LYS:HE3   | 44:YY:101:LYS:HZ3 | 1.70                     | 0.56              |
| 44:YY:95:LYS:HE3   | 44:YY:95:LYS:O    | 2.06                     | 0.56              |
| 50:Y4:50:VAL:O     | 50:Y4:51:ASP:C    | 2.48                     | 0.56              |
| 1:QA:184:G:N2      | 1:QA:193:C:O2     | 2.38                     | 0.56              |
| 1:QA:620:C:H2'     | 1:QA:621:A:O4'    | 2.06                     | 0.56              |
| 1:QA:939:G:OP1     | 7:QG:102:ARG:NH1  | 2.39                     | 0.56              |
| 7:QG:42:ILE:O      | 7:QG:117:ALA:HB2  | 2.05                     | 0.56              |
| 7:QG:73:MET:HG2    | 7:QG:90:GLU:HA    | 1.87                     | 0.56              |
| 8:QH:49:GLU:HG3    | 8:QH:51:VAL:CG1   | 2.35                     | 0.56              |
| 9:QI:114:TYR:O     | 9:QI:114:TYR:CD2  | 2.59                     | 0.56              |
| 11:QK:41:THR:HG21  | 11:QK:71:LYS:CB   | 2.36                     | 0.56              |
| 12:QL:111:LYS:O    | 12:QL:112:ASP:HB2 | 2.05                     | 0.56              |
| 13:QM:81:LEU:HB3   | 13:QM:89:GLY:HA2  | 1.88                     | 0.56              |
| 13:QM:89:GLY:O     | 13:QM:92:HIS:HB2  | 2.06                     | 0.56              |
| 25:RA:2372:G:H4'   | 52:R6:46:HIS:NE2  | 2.21                     | 0.56              |
| 26:RB:42:C:H2'     | 26:RB:43:C:O4'    | 2.05                     | 0.56              |
| 27:RD:259:THR:O    | 27:RD:260:ARG:C   | 2.49                     | 0.56              |
| 28:RE:77:ILE:O     | 28:RE:78:LEU:C    | 2.48                     | 0.56              |
| 28:RE:203:LYS:HE3  | 28:RE:204:ALA:HB2 | 1.86                     | 0.56              |
| 33:RN:131:GLN:CG   | 33:RN:132:ALA:N   | 2.68                     | 0.56              |
| 34:RO:3:GLN:CB     | 34:RO:4:PRO:HD2   | 2.35                     | 0.56              |
| 40:RU:105:VAL:HA   | 41:RV:44:LYS:HE3  | 1.88                     | 0.56              |
| 54:R8:30:ARG:O     | 54:R8:31:HIS:CB   | 2.54                     | 0.56              |
| 2:XB:7:VAL:HG22    | 2:XB:8:LYS:N      | 2.21                     | 0.56              |
| 3:XC:113:ALA:C     | 3:XC:115:LEU:H    | 2.14                     | 0.56              |
| 10:XJ:24:VAL:HG21  | 10:XJ:37:PRO:HG3  | 1.86                     | 0.56              |
| 12:XL:79:GLU:O     | 12:XL:79:GLU:HG2  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1210:A:H5'  | 25:YA:1210:A:H8    | 1.71                     | 0.56              |
| 25:YA:1697:G:H5'' | 25:YA:1698:A:H3'   | 1.88                     | 0.56              |
| 25:YA:2111:C:N3   | 25:YA:2118:U:O2'   | 2.39                     | 0.56              |
| 27:YD:94:LEU:HD13 | 27:YD:94:LEU:C     | 2.30                     | 0.56              |
| 28:YE:64:LYS:C    | 28:YE:66:HIS:H     | 2.12                     | 0.56              |
| 33:YN:40:PRO:HB3  | 40:YU:68:ALA:HB2   | 1.87                     | 0.56              |
| 35:YP:19:VAL:CG2  | 35:YP:20:GLY:H     | 1.99                     | 0.56              |
| 38:YS:5:THR:OG1   | 38:YS:7:TYR:HB3    | 2.06                     | 0.56              |
| 38:YS:14:VAL:HG13 | 38:YS:15:ARG:N     | 2.21                     | 0.56              |
| 40:YU:96:ALA:O    | 40:YU:100:VAL:HG23 | 2.05                     | 0.56              |
| 44:YY:62:GLU:O    | 44:YY:63:LYS:O     | 2.24                     | 0.56              |
| 49:Y3:59:VAL:CG1  | 49:Y3:60:GLU:N     | 2.69                     | 0.56              |
| 50:Y4:41:PRO:O    | 50:Y4:42:PHE:CB    | 2.54                     | 0.56              |
| 52:Y6:48:VAL:HG13 | 52:Y6:49:HIS:N     | 2.20                     | 0.56              |
| 2:QB:102:LEU:HB3  | 2:QB:180:LEU:CD1   | 2.36                     | 0.56              |
| 3:QC:45:LYS:HD2   | 3:QC:46:GLU:HG3    | 1.87                     | 0.56              |
| 3:QC:95:THR:CG2   | 3:QC:96:GLY:H      | 2.10                     | 0.56              |
| 3:QC:180:ALA:O    | 3:QC:181:ASN:HB3   | 2.06                     | 0.56              |
| 4:QD:52:SER:O     | 4:QD:53:ASP:C      | 2.49                     | 0.56              |
| 8:QH:19:VAL:O     | 8:QH:20:TYR:HB2    | 2.05                     | 0.56              |
| 8:QH:128:GLY:O    | 8:QH:129:VAL:HG13  | 2.06                     | 0.56              |
| 10:QJ:26:ALA:HA   | 10:QJ:29:ARG:NH2   | 2.21                     | 0.56              |
| 11:QK:125:PHE:N   | 11:QK:125:PHE:CD1  | 2.74                     | 0.56              |
| 13:QM:9:ILE:HD12  | 13:QM:9:ILE:C      | 2.31                     | 0.56              |
| 13:QM:49:THR:HB   | 13:QM:52:GLU:HG3   | 1.87                     | 0.56              |
| 13:QM:80:ARG:O    | 13:QM:84:ILE:HB    | 2.06                     | 0.56              |
| 25:RA:952:G:P     | 36:RQ:16:ARG:HH12  | 2.28                     | 0.56              |
| 27:RD:239:ARG:O   | 27:RD:240:ALA:HB2  | 2.05                     | 0.56              |
| 28:RE:64:LYS:C    | 28:RE:66:HIS:H     | 2.12                     | 0.56              |
| 31:RH:59:ARG:HH11 | 31:RH:59:ARG:CG    | 2.19                     | 0.56              |
| 35:RP:15:ARG:O    | 35:RP:17:LYS:N     | 2.39                     | 0.56              |
| 44:RY:62:GLU:O    | 44:RY:63:LYS:O     | 2.24                     | 0.56              |
| 47:R1:3:LYS:HD3   | 47:R1:43:TYR:CD2   | 2.35                     | 0.56              |
| 49:R3:7:LYS:NZ    | 49:R3:32:GLN:HE21  | 2.03                     | 0.56              |
| 50:R4:61:ARG:C    | 50:R4:63:TYR:H     | 2.14                     | 0.56              |
| 1:XA:954:G:O6     | 1:XA:1225:A:N6     | 2.39                     | 0.56              |
| 1:XA:1014:A:H4'   | 19:XS:14:HIS:HE2   | 1.69                     | 0.56              |
| 3:XC:77:ILE:O     | 3:XC:83:ARG:HB3    | 2.05                     | 0.56              |
| 4:XD:165:MET:HA   | 4:XD:165:MET:CE    | 2.36                     | 0.56              |
| 5:XE:92:LYS:O     | 5:XE:118:ILE:HD12  | 2.06                     | 0.56              |
| 7:XG:11:GLN:C     | 7:XG:12:LEU:HD22   | 2.31                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:XH:102:ARG:NH1   | 8:XH:105:ARG:NH2   | 2.54                     | 0.56              |
| 12:XL:10:LEU:HD13  | 17:XQ:32:TYR:CE2   | 2.41                     | 0.56              |
| 19:XS:65:ASN:N     | 19:XS:65:ASN:ND2   | 2.52                     | 0.56              |
| 25:YA:1021:A:H8    | 25:YA:1021:A:H3'   | 1.71                     | 0.56              |
| 27:YD:239:ARG:O    | 27:YD:240:ALA:HB2  | 2.05                     | 0.56              |
| 28:YE:55:ASN:C     | 28:YE:57:LYS:N     | 2.62                     | 0.56              |
| 30:YG:120:LEU:HB3  | 30:YG:131:TYR:OH   | 2.05                     | 0.56              |
| 30:YG:135:LEU:HD12 | 30:YG:135:LEU:N    | 2.20                     | 0.56              |
| 31:YH:126:PRO:CG   | 31:YH:127:GLU:N    | 2.65                     | 0.56              |
| 36:YQ:25:ASP:N     | 36:YQ:102:VAL:HG23 | 2.21                     | 0.56              |
| 40:YU:105:VAL:HA   | 41:YV:44:LYS:HE3   | 1.88                     | 0.56              |
| 44:YY:48:ALA:H     | 44:YY:60:PHE:HA    | 1.71                     | 0.56              |
| 49:Y3:4:LEU:HD21   | 49:Y3:39:ASP:OD1   | 2.06                     | 0.56              |
| 1:QA:596:C:N3      | 1:QA:644:G:N2      | 2.51                     | 0.55              |
| 2:QB:46:LYS:HA     | 2:QB:49:GLU:OE1    | 2.06                     | 0.55              |
| 3:QC:20:SER:CB     | 3:QC:40:ARG:HH22   | 2.14                     | 0.55              |
| 7:QG:62:PHE:HA     | 7:QG:124:LEU:CD2   | 2.27                     | 0.55              |
| 10:QJ:35:SER:O     | 10:QJ:72:VAL:HG13  | 2.06                     | 0.55              |
| 11:QK:125:PHE:HD1  | 11:QK:125:PHE:H    | 1.54                     | 0.55              |
| 14:QN:44:LEU:CD1   | 14:QN:48:ALA:HB2   | 2.36                     | 0.55              |
| 19:QS:18:LYS:O     | 19:QS:22:LEU:HD13  | 2.06                     | 0.55              |
| 21:QU:6:ARG:HH21   | 21:QU:15:ARG:HE    | 1.53                     | 0.55              |
| 25:RA:1983:C:H4'   | 25:RA:2606:C:H4'   | 1.87                     | 0.55              |
| 27:RD:155:LEU:HD23 | 27:RD:177:LEU:CD2  | 2.36                     | 0.55              |
| 31:RH:6:ARG:C      | 31:RH:8:PRO:HD2    | 2.30                     | 0.55              |
| 36:RQ:37:LEU:HD21  | 36:RQ:130:LYS:HE3  | 1.87                     | 0.55              |
| 46:R0:23:VAL:HG22  | 46:R0:38:VAL:HG22  | 1.88                     | 0.55              |
| 2:XB:68:ILE:HD12   | 2:XB:68:ILE:N      | 2.21                     | 0.55              |
| 2:XB:217:ARG:HA    | 2:XB:220:ASP:OD2   | 2.06                     | 0.55              |
| 4:XD:28:SER:CB     | 4:XD:29:PRO:CD     | 2.84                     | 0.55              |
| 4:XD:52:SER:O      | 4:XD:53:ASP:C      | 2.49                     | 0.55              |
| 5:XE:107:ARG:O     | 5:XE:108:ALA:C     | 2.49                     | 0.55              |
| 6:XF:41:GLU:HG2    | 6:XF:43:LEU:HD11   | 1.89                     | 0.55              |
| 8:XH:49:GLU:O      | 8:XH:51:VAL:N      | 2.39                     | 0.55              |
| 11:XK:41:THR:HG21  | 11:XK:71:LYS:CB    | 2.36                     | 0.55              |
| 12:XL:83:VAL:HG22  | 12:XL:84:LEU:N     | 2.21                     | 0.55              |
| 15:XO:24:SER:O     | 15:XO:28:GLN:HG3   | 2.06                     | 0.55              |
| 16:XP:53:VAL:HG23  | 16:XP:54:GLU:H     | 1.70                     | 0.55              |
| 25:YA:458:G:O2'    | 53:Y7:39:ARG:HD3   | 2.06                     | 0.55              |
| 25:YA:1824:G:O3'   | 27:YD:249:PRO:HD3  | 2.06                     | 0.55              |
| 28:YE:117:MET:O    | 28:YE:117:MET:HG3  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:YF:198:ALA:CA  | 29:YF:201:VAL:HG12 | 2.34                     | 0.55              |
| 35:YP:31:ALA:C    | 35:YP:32:THR:HG23  | 2.31                     | 0.55              |
| 43:YX:18:TYR:C    | 43:YX:20:GLY:N     | 2.64                     | 0.55              |
| 48:Y2:43:GLN:O    | 48:Y2:44:LEU:CG    | 2.54                     | 0.55              |
| 51:Y5:20:ARG:C    | 51:Y5:22:HIS:H     | 2.14                     | 0.55              |
| 52:Y6:11:LEU:HD23 | 52:Y6:26:ASN:HB3   | 1.87                     | 0.55              |
| 2:QB:204:ASN:HD22 | 2:QB:205:ASP:N     | 2.04                     | 0.55              |
| 3:QC:113:ALA:C    | 3:QC:115:LEU:H     | 2.14                     | 0.55              |
| 7:QG:46:ALA:HB2   | 7:QG:117:ALA:HB1   | 1.88                     | 0.55              |
| 7:QG:148:ASN:N    | 7:QG:148:ASN:ND2   | 2.46                     | 0.55              |
| 8:QH:82:HIS:HD2   | 8:QH:83:ILE:N      | 2.03                     | 0.55              |
| 16:QP:59:TRP:HA   | 16:QP:59:TRP:CE3   | 2.42                     | 0.55              |
| 25:RA:2150:U:H2'  | 25:RA:2151:G:C8    | 2.42                     | 0.55              |
| 27:RD:31:LYS:O    | 27:RD:35:LYS:O     | 2.24                     | 0.55              |
| 27:RD:35:LYS:NZ   | 27:RD:64:ILE:O     | 2.32                     | 0.55              |
| 40:RU:83:LEU:HD12 | 40:RU:113:ALA:HB2  | 1.86                     | 0.55              |
| 42:RW:14:PRO:HG2  | 42:RW:78:GLU:OE2   | 2.07                     | 0.55              |
| 1:XA:234:C:H2'    | 1:XA:235:C:C6      | 2.42                     | 0.55              |
| 1:XA:1129:C:H5'   | 1:XA:1130:A:OP1    | 2.06                     | 0.55              |
| 8:XH:128:GLY:O    | 8:XH:129:VAL:HG13  | 2.06                     | 0.55              |
| 10:XJ:26:ALA:HA   | 10:XJ:29:ARG:NH2   | 2.21                     | 0.55              |
| 12:XL:58:VAL:O    | 12:XL:65:GLU:HA    | 2.06                     | 0.55              |
| 16:XP:43:LYS:C    | 16:XP:45:THR:H     | 2.14                     | 0.55              |
| 17:XQ:6:LEU:O     | 17:XQ:58:GLU:HA    | 2.05                     | 0.55              |
| 19:XS:18:LYS:O    | 19:XS:22:LEU:HD13  | 2.06                     | 0.55              |
| 20:XT:94:ALA:O    | 20:XT:95:ALA:CB    | 2.54                     | 0.55              |
| 21:XU:6:ARG:O     | 21:XU:8:THR:N      | 2.39                     | 0.55              |
| 25:YA:1309:G:OP1  | 53:Y7:9:ARG:HD3    | 2.06                     | 0.55              |
| 25:YA:2698:U:H2'  | 25:YA:2699:C:C6    | 2.41                     | 0.55              |
| 27:YD:35:LYS:NZ   | 27:YD:64:ILE:O     | 2.32                     | 0.55              |
| 29:YF:198:ALA:C   | 29:YF:200:GLU:N    | 2.62                     | 0.55              |
| 35:YP:14:LYS:O    | 35:YP:16:ARG:N     | 2.39                     | 0.55              |
| 36:YQ:63:LYS:HD2  | 45:YZ:175:VAL:HG21 | 1.87                     | 0.55              |
| 39:YT:107:ASP:O   | 39:YT:111:ARG:NH1  | 2.39                     | 0.55              |
| 49:Y3:8:LEU:HD22  | 49:Y3:31:LEU:CD2   | 2.36                     | 0.55              |
| 1:QA:501:C:H2'    | 1:QA:502:G:C8      | 2.41                     | 0.55              |
| 5:QE:7:GLU:HG2    | 5:QE:112:LEU:HD22  | 1.88                     | 0.55              |
| 5:QE:126:ARG:HG3  | 5:QE:126:ARG:NH1   | 2.19                     | 0.55              |
| 19:QS:9:VAL:HG23  | 19:QS:9:VAL:O      | 2.04                     | 0.55              |
| 25:RA:2126:A:H4'  | 25:RA:2127:G:O5'   | 2.06                     | 0.55              |
| 26:RB:33:G:P      | 30:RG:2:PRO:HG3    | 2.47                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:RD:94:LEU:HD13 | 27:RD:94:LEU:C    | 2.31                     | 0.55              |
| 28:RE:4:ILE:HD13  | 28:RE:5:LEU:H     | 1.71                     | 0.55              |
| 34:RO:79:PHE:HD2  | 39:RT:72:VAL:HG22 | 1.72                     | 0.55              |
| 35:RP:39:LYS:CA   | 35:RP:45:LEU:CD1  | 2.80                     | 0.55              |
| 44:RY:95:LYS:HB2  | 44:RY:95:LYS:NZ   | 2.21                     | 0.55              |
| 1:XA:15:G:H4'     | 5:XE:24:ARG:HH12  | 1.71                     | 0.55              |
| 1:XA:31:G:O2'     | 1:XA:48:C:N4      | 2.37                     | 0.55              |
| 1:XA:54:C:N4      | 1:XA:353:A:OP2    | 2.36                     | 0.55              |
| 1:XA:963:G:H21    | 10:XJ:55:LYS:HD3  | 1.72                     | 0.55              |
| 1:XA:986:A:N3     | 19:XS:52:TYR:OH   | 2.38                     | 0.55              |
| 1:XA:1502:A:H2    | 1:XA:1505:G:H1    | 1.53                     | 0.55              |
| 2:XB:41:ILE:HD12  | 2:XB:41:ILE:N     | 2.21                     | 0.55              |
| 2:XB:96:ARG:H     | 2:XB:96:ARG:CD    | 2.17                     | 0.55              |
| 2:XB:204:ASN:HD22 | 2:XB:205:ASP:N    | 2.04                     | 0.55              |
| 3:XC:59:ARG:NH2   | 3:XC:97:LYS:HE3   | 2.20                     | 0.55              |
| 3:XC:112:SER:OG   | 3:XC:115:LEU:HG   | 2.06                     | 0.55              |
| 5:XE:144:THR:O    | 5:XE:148:VAL:HG23 | 2.06                     | 0.55              |
| 7:XG:50:ILE:CB    | 7:XG:58:PRO:HB3   | 2.37                     | 0.55              |
| 19:XS:40:ILE:HG12 | 19:XS:41:VAL:N    | 2.20                     | 0.55              |
| 25:YA:2263:C:H2'  | 25:YA:2264:C:H6   | 1.71                     | 0.55              |
| 33:YN:131:GLN:CG  | 33:YN:132:ALA:N   | 2.68                     | 0.55              |
| 35:YP:13:ASN:O    | 35:YP:14:LYS:C    | 2.49                     | 0.55              |
| 36:YQ:12:GLN:OE1  | 36:YQ:72:LYS:HD2  | 2.06                     | 0.55              |
| 37:YR:84:ALA:HB3  | 37:YR:85:PRO:HD3  | 1.88                     | 0.55              |
| 40:YU:92:ARG:NH1  | 41:YV:11:GLN:HB2  | 2.22                     | 0.55              |
| 44:YY:84:ARG:NH1  | 44:YY:97:ARG:HB2  | 2.11                     | 0.55              |
| 44:YY:89:PHE:O    | 44:YY:90:LEU:HD13 | 2.05                     | 0.55              |
| 44:YY:91:GLU:HG3  | 44:YY:92:ASN:H    | 1.71                     | 0.55              |
| 47:Y1:4:VAL:HG23  | 47:Y1:10:LYS:C    | 2.32                     | 0.55              |
| 47:Y1:91:LYS:CG   | 47:Y1:92:LYS:H    | 2.15                     | 0.55              |
| 48:Y2:15:LYS:H    | 48:Y2:67:LYS:NZ   | 2.03                     | 0.55              |
| 49:Y3:35:ARG:HB3  | 49:Y3:37:LEU:CD2  | 2.37                     | 0.55              |
| 1:QA:280:C:C2     | 17:QQ:38:ARG:HG3  | 2.42                     | 0.55              |
| 2:QB:217:ARG:HA   | 2:QB:220:ASP:OD2  | 2.06                     | 0.55              |
| 3:QC:112:SER:OG   | 3:QC:115:LEU:HG   | 2.06                     | 0.55              |
| 6:QF:89:MET:HE1   | 18:QR:76:LEU:CD2  | 2.36                     | 0.55              |
| 11:QK:34:ASP:N    | 11:QK:40:ILE:HD11 | 2.20                     | 0.55              |
| 11:QK:50:TYR:HH   | 11:QK:59:TYR:HE2  | 1.54                     | 0.55              |
| 15:QO:8:LYS:HB2   | 15:QO:8:LYS:HZ2   | 1.68                     | 0.55              |
| 16:QP:48:TRP:O    | 16:QP:49:LEU:HB2  | 2.06                     | 0.55              |
| 25:RA:643:A:N1    | 25:RA:2369:A:O2'  | 2.40                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2006:C:O2'  | 25:RA:2823:A:N3    | 2.38                     | 0.55              |
| 27:RD:36:PRO:HB2  | 27:RD:61:LEU:HG    | 1.87                     | 0.55              |
| 27:RD:69:ARG:HD3  | 27:RD:105:ILE:HD11 | 1.87                     | 0.55              |
| 29:RF:28:ILE:HD12 | 29:RF:28:ILE:O     | 2.06                     | 0.55              |
| 38:RS:14:VAL:HG13 | 38:RS:15:ARG:N     | 2.21                     | 0.55              |
| 41:RV:49:THR:CB   | 41:RV:50:PRO:HD2   | 2.25                     | 0.55              |
| 45:RZ:35:ARG:HH11 | 45:RZ:35:ARG:HB3   | 1.71                     | 0.55              |
| 47:R1:4:VAL:HG23  | 47:R1:10:LYS:C     | 2.32                     | 0.55              |
| 49:R3:4:LEU:HD21  | 49:R3:39:ASP:OD1   | 2.06                     | 0.55              |
| 54:R8:63:PRO:O    | 54:R8:64:TYR:HB2   | 2.07                     | 0.55              |
| 1:XA:8:A:N6       | 4:XD:205:GLU:O     | 2.39                     | 0.55              |
| 1:XA:880:C:OP1    | 12:XL:8:ASN:ND2    | 2.38                     | 0.55              |
| 1:XA:1218:C:H2'   | 1:XA:1219:U:C6     | 2.42                     | 0.55              |
| 1:XA:1347:G:N7    | 9:XI:11:LYS:NZ     | 2.53                     | 0.55              |
| 2:XB:214:ILE:HA   | 2:XB:217:ARG:NH2   | 2.21                     | 0.55              |
| 3:XC:6:HIS:CD2    | 3:XC:7:PRO:HD2     | 2.41                     | 0.55              |
| 3:XC:45:LYS:HD2   | 3:XC:46:GLU:HG3    | 1.87                     | 0.55              |
| 3:XC:188:LEU:N    | 3:XC:188:LEU:HD22  | 2.21                     | 0.55              |
| 12:XL:27:LEU:C    | 12:XL:29:GLY:N     | 2.64                     | 0.55              |
| 25:YA:1859:A:N6   | 25:YA:1883:G:O2'   | 2.40                     | 0.55              |
| 28:YE:3:GLY:HA3   | 28:YE:81:ILE:HD12  | 1.88                     | 0.55              |
| 29:YF:29:ASN:N    | 29:YF:112:MET:HE1  | 2.19                     | 0.55              |
| 31:YH:152:ARG:C   | 31:YH:153:LYS:HE2  | 2.32                     | 0.55              |
| 35:YP:15:ARG:O    | 35:YP:17:LYS:N     | 2.39                     | 0.55              |
| 35:YP:31:ALA:O    | 35:YP:32:THR:HG23  | 2.05                     | 0.55              |
| 38:YS:18:ILE:C    | 38:YS:19:LYS:O     | 2.44                     | 0.55              |
| 38:YS:59:LYS:CG   | 38:YS:60:GLY:H     | 2.11                     | 0.55              |
| 40:YU:73:GLY:O    | 40:YU:74:LEU:HB3   | 2.07                     | 0.55              |
| 42:YW:14:PRO:HG2  | 42:YW:78:GLU:OE2   | 2.07                     | 0.55              |
| 2:QB:169:LYS:HD3  | 2:QB:169:LYS:O     | 2.06                     | 0.55              |
| 5:QE:144:THR:O    | 5:QE:148:VAL:HG23  | 2.06                     | 0.55              |
| 7:QG:20:ASP:HB3   | 7:QG:23:VAL:HG23   | 1.88                     | 0.55              |
| 9:QI:82:ALA:O     | 9:QI:86:VAL:HB     | 2.06                     | 0.55              |
| 13:QM:30:ALA:O    | 13:QM:31:LYS:C     | 2.49                     | 0.55              |
| 15:QO:65:ARG:HB2  | 15:QO:65:ARG:NH1   | 2.20                     | 0.55              |
| 16:QP:53:VAL:HG23 | 16:QP:54:GLU:H     | 1.71                     | 0.55              |
| 25:RA:49:A:N7     | 25:RA:120:U:H5     | 2.05                     | 0.55              |
| 25:RA:307:G:N1    | 25:RA:310:A:OP2    | 2.37                     | 0.55              |
| 25:RA:2250:G:C5   | 36:RQ:82:ARG:HD2   | 2.42                     | 0.55              |
| 26:RB:43:C:N4     | 26:RB:45:A:N1      | 2.54                     | 0.55              |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:CZ    | 2.42                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:67:PHE:O     | 28:RE:69:LYS:N     | 2.39                     | 0.55              |
| 31:RH:152:ARG:C    | 31:RH:153:LYS:HE2  | 2.32                     | 0.55              |
| 34:RO:68:GLU:HA    | 34:RO:78:ARG:HB3   | 1.89                     | 0.55              |
| 35:RP:115:LEU:HD12 | 35:RP:116:GLY:N    | 2.21                     | 0.55              |
| 40:RU:104:GLN:OE1  | 40:RU:104:GLN:N    | 2.35                     | 0.55              |
| 41:RV:52:VAL:O     | 41:RV:54:GLY:N     | 2.39                     | 0.55              |
| 42:RW:88:ARG:HB3   | 42:RW:92:ARG:HB3   | 1.88                     | 0.55              |
| 44:RY:21:LYS:HG3   | 44:RY:22:GLY:H     | 1.69                     | 0.55              |
| 50:R4:9:LEU:H      | 50:R4:27:THR:HG22  | 1.71                     | 0.55              |
| 1:XA:918:A:H2'     | 1:XA:919:A:C8      | 2.41                     | 0.55              |
| 4:XD:126:ILE:HG22  | 4:XD:127:THR:N     | 2.22                     | 0.55              |
| 5:XE:99:GLY:O      | 5:XE:117:ASP:HA    | 2.06                     | 0.55              |
| 6:XF:33:TYR:HE2    | 6:XF:74:ASP:HB3    | 1.71                     | 0.55              |
| 10:XJ:4:ILE:CB     | 10:XJ:74:ILE:HD11  | 2.36                     | 0.55              |
| 11:XK:125:PHE:N    | 11:XK:125:PHE:CD1  | 2.74                     | 0.55              |
| 20:XT:43:LEU:HA    | 20:XT:46:GLU:HB3   | 1.89                     | 0.55              |
| 20:XT:53:LEU:HA    | 20:XT:56:MET:HB3   | 1.87                     | 0.55              |
| 21:XU:21:TYR:O     | 21:XU:22:ARG:HB2   | 2.05                     | 0.55              |
| 25:YA:24:G:O2'     | 42:YW:78:GLU:O     | 2.23                     | 0.55              |
| 25:YA:265:A:O2'    | 25:YA:266:G:H4'    | 2.06                     | 0.55              |
| 25:YA:857:C:OP2    | 46:Y0:77:ARG:NH2   | 2.39                     | 0.55              |
| 34:YO:4:PRO:O      | 34:YO:5:GLN:HB2    | 2.05                     | 0.55              |
| 35:YP:39:LYS:N     | 35:YP:45:LEU:HD11  | 2.21                     | 0.55              |
| 35:YP:49:ARG:NE    | 54:Y8:59:LYS:HG2   | 2.22                     | 0.55              |
| 44:YY:61:ILE:HG23  | 44:YY:62:GLU:H     | 1.71                     | 0.55              |
| 50:Y4:61:ARG:C     | 50:Y4:63:TYR:H     | 2.14                     | 0.55              |
| 52:Y6:42:TRP:N     | 52:Y6:42:TRP:CD1   | 2.73                     | 0.55              |
| 4:QD:126:ILE:HG22  | 4:QD:127:THR:N     | 2.22                     | 0.55              |
| 8:QH:49:GLU:O      | 8:QH:51:VAL:N      | 2.39                     | 0.55              |
| 9:QI:45:ALA:O      | 9:QI:48:GLU:HG2    | 2.07                     | 0.55              |
| 10:QJ:6:ILE:CG2    | 10:QJ:98:ILE:HG13  | 2.21                     | 0.55              |
| 17:QQ:13:ASP:C     | 17:QQ:15:MET:H     | 2.15                     | 0.55              |
| 19:QS:7:LYS:HG3    | 19:QS:8:GLY:N      | 2.22                     | 0.55              |
| 19:QS:41:VAL:CB    | 19:QS:42:PRO:CA    | 2.76                     | 0.55              |
| 25:RA:1826:G:H4'   | 27:RD:242:ARG:NH2  | 2.17                     | 0.55              |
| 25:RA:2123:G:H2'   | 25:RA:2124:G:H8    | 1.72                     | 0.55              |
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:H    | 1.71                     | 0.55              |
| 30:RG:114:ILE:HD11 | 30:RG:140:ILE:HD12 | 1.89                     | 0.55              |
| 31:RH:151:ILE:C    | 31:RH:152:ARG:O    | 2.49                     | 0.55              |
| 35:RP:104:GLY:C    | 35:RP:105:LEU:HD12 | 2.31                     | 0.55              |
| 40:RU:27:LEU:O     | 40:RU:29:SER:N     | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:RY:48:ALA:H     | 44:RY:60:PHE:HA    | 1.71                     | 0.55              |
| 44:RY:88:LYS:HA    | 44:RY:88:LYS:HZ2   | 1.72                     | 0.55              |
| 45:RZ:104:PHE:HD1  | 45:RZ:139:VAL:HB   | 1.71                     | 0.55              |
| 50:R4:65:ASP:O     | 50:R4:66:SER:HB3   | 2.07                     | 0.55              |
| 1:XA:64:G:N2       | 1:XA:68:G:O6       | 2.37                     | 0.55              |
| 1:XA:626:U:H2'     | 1:XA:627:G:H8      | 1.71                     | 0.55              |
| 2:XB:46:LYS:HA     | 2:XB:49:GLU:OE1    | 2.05                     | 0.55              |
| 4:XD:10:ARG:HH11   | 4:XD:10:ARG:HG3    | 1.72                     | 0.55              |
| 8:XH:102:ARG:NH1   | 8:XH:105:ARG:NH1   | 2.55                     | 0.55              |
| 9:XI:82:ALA:O      | 9:XI:86:VAL:HB     | 2.06                     | 0.55              |
| 11:XK:20:TYR:HB2   | 11:XK:31:THR:O     | 2.07                     | 0.55              |
| 13:XM:9:ILE:HD12   | 13:XM:9:ILE:C      | 2.31                     | 0.55              |
| 15:XO:65:ARG:HB2   | 15:XO:65:ARG:NH1   | 2.20                     | 0.55              |
| 16:XP:59:TRP:HA    | 16:XP:59:TRP:CE3   | 2.41                     | 0.55              |
| 17:XQ:50:LYS:HG3   | 17:XQ:51:TYR:CE1   | 2.41                     | 0.55              |
| 25:YA:389:G:N1     | 35:YP:71:VAL:HG12  | 2.22                     | 0.55              |
| 25:YA:1416:G:N2    | 25:YA:1582:C:O2    | 2.38                     | 0.55              |
| 25:YA:1688:U:O2    | 25:YA:1700:A:H5''  | 2.06                     | 0.55              |
| 25:YA:2277:G:OP2   | 46:Y0:10:THR:HG21  | 2.07                     | 0.55              |
| 27:YD:43:ARG:CB    | 27:YD:54:ARG:HB2   | 2.37                     | 0.55              |
| 27:YD:94:LEU:HD22  | 27:YD:95:LEU:H     | 1.69                     | 0.55              |
| 28:YE:4:ILE:HD13   | 28:YE:5:LEU:H      | 1.71                     | 0.55              |
| 32:YI:73:GLU:HG3   | 32:YI:136:VAL:HG23 | 1.89                     | 0.55              |
| 36:YQ:64:ILE:HA    | 36:YQ:106:VAL:CG1  | 2.33                     | 0.55              |
| 40:YU:6:THR:O      | 40:YU:9:VAL:HG23   | 2.07                     | 0.55              |
| 4:QD:107:ARG:C     | 4:QD:109:GLY:H     | 2.14                     | 0.55              |
| 8:QH:23:SER:HB2    | 8:QH:61:VAL:O      | 2.07                     | 0.55              |
| 13:QM:82:MET:O     | 13:QM:83:ASP:C     | 2.49                     | 0.55              |
| 14:QN:22:THR:HB    | 14:QN:33:VAL:HG11  | 1.88                     | 0.55              |
| 17:QQ:62:SER:HB3   | 17:QQ:72:ARG:HH21  | 1.72                     | 0.55              |
| 25:RA:623:G:H2'    | 25:RA:624:C:C6     | 2.42                     | 0.55              |
| 25:RA:828:U:H4'    | 25:RA:831:G:N1     | 2.22                     | 0.55              |
| 25:RA:1009:A:OP2   | 25:RA:1010:A:OP2   | 2.24                     | 0.55              |
| 25:RA:1332:G:N2    | 25:RA:1609:A:HO2'  | 2.04                     | 0.55              |
| 27:RD:2:ALA:O      | 27:RD:3:VAL:HB     | 2.06                     | 0.55              |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:H    | 1.72                     | 0.55              |
| 29:RF:118:ALA:O    | 29:RF:121:GLY:N    | 2.33                     | 0.55              |
| 29:RF:129:PHE:O    | 29:RF:130:ALA:CB   | 2.55                     | 0.55              |
| 30:RG:7:LEU:HD12   | 30:RG:104:GLU:HA   | 1.88                     | 0.55              |
| 33:RN:109:LYS:N    | 33:RN:109:LYS:HD2  | 2.22                     | 0.55              |
| 35:RP:2:LYS:O      | 35:RP:5:ASP:HB2    | 2.06                     | 0.55              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:RQ:25:ASP:N      | 36:RQ:102:VAL:HG23 | 2.21                     | 0.55              |
| 38:RS:18:ILE:C      | 38:RS:19:LYS:O     | 2.44                     | 0.55              |
| 38:RS:36:TYR:HD2    | 38:RS:52:SER:CB    | 2.19                     | 0.55              |
| 40:RU:58:ARG:O      | 40:RU:62:ILE:HG13  | 2.06                     | 0.55              |
| 47:R1:80:LEU:C      | 47:R1:81:LYS:CE    | 2.77                     | 0.55              |
| 48:R2:41:ILE:HD11   | 48:R2:44:LEU:CG    | 2.36                     | 0.55              |
| 1:XA:520:A:O2'      | 12:XL:73:GLU:HG2   | 2.07                     | 0.55              |
| 6:XF:52:ILE:O       | 6:XF:53:ALA:HB3    | 2.07                     | 0.55              |
| 8:XH:23:SER:HB2     | 8:XH:61:VAL:O      | 2.07                     | 0.55              |
| 9:XI:126:SER:O      | 9:XI:128:ARG:N     | 2.35                     | 0.55              |
| 10:XJ:16:LEU:HD13   | 10:XJ:16:LEU:O     | 2.07                     | 0.55              |
| 12:XL:28:LYS:O      | 12:XL:29:GLY:C     | 2.50                     | 0.55              |
| 15:XO:39:LEU:O      | 15:XO:40:SER:C     | 2.50                     | 0.55              |
| 17:XQ:13:ASP:C      | 17:XQ:15:MET:H     | 2.15                     | 0.55              |
| 25:YA:1142(A):A:H4' | 33:YN:25:ARG:NH2   | 2.18                     | 0.55              |
| 25:YA:2776:A:OP1    | 25:YA:2776:A:H3'   | 2.06                     | 0.55              |
| 26:YB:40:U:O2'      | 26:YB:45:A:N6      | 2.36                     | 0.55              |
| 26:YB:49:C:H2'      | 26:YB:50:G:C8      | 2.42                     | 0.55              |
| 28:YE:20:ALA:O      | 28:YE:21:VAL:CG2   | 2.49                     | 0.55              |
| 28:YE:21:VAL:HG23   | 28:YE:22:PRO:HD3   | 1.89                     | 0.55              |
| 29:YF:24:LEU:HB3    | 29:YF:115:ALA:HB2  | 1.87                     | 0.55              |
| 30:YG:34:LEU:HD11   | 30:YG:99:MET:HE2   | 1.88                     | 0.55              |
| 34:YO:20:MET:HG2    | 34:YO:21:CYS:N     | 2.19                     | 0.55              |
| 39:YT:16:ARG:HG2    | 39:YT:18:ASP:OD1   | 2.06                     | 0.55              |
| 41:YV:29:PRO:HA     | 41:YV:61:VAL:CG2   | 2.37                     | 0.55              |
| 47:Y1:83:GLU:CD     | 47:Y1:85:LEU:H     | 2.15                     | 0.55              |
| 47:Y1:92:LYS:C      | 47:Y1:94:LEU:N     | 2.62                     | 0.55              |
| 50:Y4:9:LEU:H       | 50:Y4:27:THR:HG22  | 1.71                     | 0.55              |
| 51:Y5:55:ARG:HD3    | 51:Y5:56:LYS:N     | 2.21                     | 0.55              |
| 5:QE:92:LYS:O       | 5:QE:118:ILE:HD12  | 2.06                     | 0.55              |
| 7:QG:50:ILE:HG22    | 7:QG:50:ILE:O      | 2.07                     | 0.55              |
| 10:QJ:84:GLN:C      | 10:QJ:86:MET:H     | 2.14                     | 0.55              |
| 12:QL:79:GLU:HG2    | 12:QL:79:GLU:O     | 2.06                     | 0.55              |
| 25:RA:2030:A:H4'    | 25:RA:2031:A:C8    | 2.41                     | 0.55              |
| 26:RB:11:C:H3'      | 26:RB:12:C:C6      | 2.42                     | 0.55              |
| 28:RE:3:GLY:HA3     | 28:RE:81:ILE:HD12  | 1.88                     | 0.55              |
| 30:RG:3:LEU:HD12    | 30:RG:4:ASP:N      | 2.19                     | 0.55              |
| 30:RG:135:LEU:HD12  | 30:RG:135:LEU:N    | 2.21                     | 0.55              |
| 31:RH:143:GLN:HE21  | 31:RH:143:GLN:C    | 2.15                     | 0.55              |
| 35:RP:39:LYS:N      | 35:RP:45:LEU:HD11  | 2.21                     | 0.55              |
| 37:RR:12:ARG:HH11   | 37:RR:12:ARG:HG3   | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:RU:74:LEU:HD13  | 40:RU:79:PHE:HB2   | 1.89                     | 0.55              |
| 40:RU:92:ARG:NH1   | 41:RV:11:GLN:HB2   | 2.22                     | 0.55              |
| 54:R8:56:GLU:O     | 54:R8:57:ARG:C     | 2.50                     | 0.55              |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:C8  | 2.41                     | 0.55              |
| 1:XA:1316:G:N1     | 1:XA:1319:A:OP2    | 2.40                     | 0.55              |
| 1:XA:1333:A:H2'    | 1:XA:1334:G:O4'    | 2.07                     | 0.55              |
| 7:XG:73:MET:HG2    | 7:XG:90:GLU:HA     | 1.88                     | 0.55              |
| 9:XI:45:ALA:O      | 9:XI:48:GLU:HG2    | 2.07                     | 0.55              |
| 10:XJ:19:SER:O     | 10:XJ:23:ILE:HG13  | 2.07                     | 0.55              |
| 10:XJ:81:THR:C     | 10:XJ:83:GLU:N     | 2.64                     | 0.55              |
| 10:XJ:84:GLN:C     | 10:XJ:86:MET:H     | 2.14                     | 0.55              |
| 11:XK:125:PHE:HD1  | 11:XK:125:PHE:H    | 1.54                     | 0.55              |
| 13:XM:3:ARG:HH21   | 30:YG:139:LEU:HD13 | 1.71                     | 0.55              |
| 13:XM:81:LEU:HB3   | 13:XM:89:GLY:HA2   | 1.88                     | 0.55              |
| 18:XR:58:LEU:HD12  | 18:XR:58:LEU:H     | 1.72                     | 0.55              |
| 25:YA:593:G:O2'    | 54:Y8:61:LEU:HD13  | 2.06                     | 0.55              |
| 25:YA:1251:C:OP1   | 40:YU:10:ARG:HG3   | 2.07                     | 0.55              |
| 25:YA:1301:A:O2'   | 25:YA:1302:A:H3'   | 2.07                     | 0.55              |
| 25:YA:2224:G:OP1   | 27:YD:268:ARG:HD3  | 2.07                     | 0.55              |
| 28:YE:53:PRO:O     | 28:YE:74:PRO:HA    | 2.07                     | 0.55              |
| 29:YF:28:ILE:HD12  | 29:YF:28:ILE:O     | 2.06                     | 0.55              |
| 31:YH:143:GLN:C    | 31:YH:143:GLN:HE21 | 2.15                     | 0.55              |
| 33:YN:44:PRO:HG2   | 33:YN:45:ASN:H     | 1.71                     | 0.55              |
| 34:YO:79:PHE:HD2   | 39:YT:72:VAL:HG22  | 1.72                     | 0.55              |
| 36:YQ:21:THR:O     | 36:YQ:22:LYS:O     | 2.25                     | 0.55              |
| 38:YS:107:GLU:N    | 38:YS:110:LEU:HD11 | 2.22                     | 0.55              |
| 39:YT:123:GLN:O    | 39:YT:125:ARG:N    | 2.40                     | 0.55              |
| 40:YU:58:ARG:O     | 40:YU:62:ILE:HG13  | 2.06                     | 0.55              |
| 42:YW:25:ARG:HH11  | 42:YW:25:ARG:CB    | 2.20                     | 0.55              |
| 50:Y4:48:ARG:HH12  | 50:Y4:52:THR:HG22  | 1.71                     | 0.55              |
| 50:Y4:71:ARG:NH1   | 50:Y4:71:ARG:CG    | 2.61                     | 0.55              |
| 53:Y7:19:ARG:HH11  | 53:Y7:19:ARG:HG2   | 1.71                     | 0.55              |
| 1:QA:381:C:H2'     | 1:QA:382:A:O4'     | 2.06                     | 0.55              |
| 3:QC:11:ARG:HH21   | 3:QC:180:ALA:HB3   | 1.70                     | 0.55              |
| 3:QC:188:LEU:N     | 3:QC:188:LEU:HD22  | 2.22                     | 0.55              |
| 8:QH:102:ARG:HH11  | 8:QH:105:ARG:CZ    | 2.19                     | 0.55              |
| 9:QI:40:LEU:HD11   | 9:QI:70:LYS:CG     | 2.37                     | 0.55              |
| 10:QJ:16:LEU:HD13  | 10:QJ:16:LEU:O     | 2.07                     | 0.55              |
| 10:QJ:32:ALA:O     | 10:QJ:33:GLN:O     | 2.25                     | 0.55              |
| 15:QO:29:VAL:HG11  | 15:QO:67:LEU:HD21  | 1.89                     | 0.55              |
| 15:QO:77:ARG:HA    | 15:QO:80:ALA:CB    | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:QR:30:ASP:C     | 18:QR:32:ARG:H     | 2.15                     | 0.55              |
| 25:RA:181:A:H1'    | 25:RA:435:C:H5'    | 1.88                     | 0.55              |
| 25:RA:1416:G:H2'   | 25:RA:1417:C:C6    | 2.42                     | 0.55              |
| 27:RD:65:ILE:HD13  | 27:RD:65:ILE:C     | 2.32                     | 0.55              |
| 29:RF:147:GLY:O    | 29:RF:148:LEU:HD23 | 2.07                     | 0.55              |
| 33:RN:87:LEU:HD23  | 33:RN:87:LEU:C     | 2.32                     | 0.55              |
| 40:RU:73:GLY:O     | 40:RU:74:LEU:HB3   | 2.07                     | 0.55              |
| 41:RV:29:PRO:HA    | 41:RV:61:VAL:CG2   | 2.37                     | 0.55              |
| 41:RV:99:ILE:N     | 41:RV:99:ILE:CD1   | 2.65                     | 0.55              |
| 45:RZ:166:SER:HB2  | 45:RZ:168:GLU:N    | 2.22                     | 0.55              |
| 1:XA:719:C:O2'     | 18:XR:49:LYS:HB3   | 2.07                     | 0.55              |
| 1:XA:1112:C:H1'    | 3:XC:179:ARG:NH1   | 2.21                     | 0.55              |
| 2:XB:170:GLU:HA    | 2:XB:172:ILE:HD12  | 1.89                     | 0.55              |
| 4:XD:31:CYS:O      | 4:XD:32:ALA:HB3    | 2.07                     | 0.55              |
| 4:XD:94:LEU:H      | 4:XD:94:LEU:CD1    | 2.08                     | 0.55              |
| 5:XE:7:GLU:HG2     | 5:XE:112:LEU:HD22  | 1.88                     | 0.55              |
| 6:XF:92:LYS:HB2    | 6:XF:92:LYS:NZ     | 2.22                     | 0.55              |
| 14:XN:8:GLU:C      | 14:XN:10:ALA:H     | 2.14                     | 0.55              |
| 17:XQ:48:GLU:O     | 17:XQ:49:GLU:C     | 2.49                     | 0.55              |
| 22:XV:68:C:H2'     | 22:XV:69:C:C6      | 2.42                     | 0.55              |
| 25:YA:395:U:H2'    | 25:YA:396:G:N7     | 2.22                     | 0.55              |
| 25:YA:2466:C:OP1   | 55:Y9:4:ARG:HB2    | 2.07                     | 0.55              |
| 28:YE:67:PHE:O     | 28:YE:69:LYS:N     | 2.39                     | 0.55              |
| 30:YG:114:ILE:HD11 | 30:YG:140:ILE:HD12 | 1.89                     | 0.55              |
| 33:YN:87:LEU:HD23  | 33:YN:87:LEU:C     | 2.32                     | 0.55              |
| 33:YN:109:LYS:N    | 33:YN:109:LYS:HD2  | 2.22                     | 0.55              |
| 34:YO:19:ILE:O     | 34:YO:19:ILE:HD13  | 2.06                     | 0.55              |
| 35:YP:2:LYS:O      | 35:YP:5:ASP:HB2    | 2.06                     | 0.55              |
| 39:YT:29:ARG:HH11  | 39:YT:29:ARG:HB2   | 1.72                     | 0.55              |
| 44:YY:95:LYS:HD3   | 44:YY:95:LYS:N     | 2.22                     | 0.55              |
| 50:Y4:37:SER:C     | 50:Y4:39:CYS:N     | 2.62                     | 0.55              |
| 7:QG:11:GLN:C      | 7:QG:12:LEU:HD22   | 2.31                     | 0.55              |
| 7:QG:37:ASN:HD21   | 9:QI:40:LEU:HD23   | 1.69                     | 0.55              |
| 12:QL:83:VAL:HG22  | 12:QL:84:LEU:N     | 2.21                     | 0.55              |
| 25:RA:2420:C:N4    | 54:R8:30:ARG:HD2   | 2.21                     | 0.55              |
| 25:RA:2667:C:H1'   | 31:RH:109:PHE:CD2  | 2.40                     | 0.55              |
| 25:RA:2724:C:P     | 37:RR:1:MET:HE3    | 2.47                     | 0.55              |
| 31:RH:128:PRO:CD   | 31:RH:129:THR:N    | 2.70                     | 0.55              |
| 35:RP:106:LEU:O    | 35:RP:107:LYS:HD3  | 2.07                     | 0.55              |
| 38:RS:13:ARG:O     | 38:RS:13:ARG:HD2   | 2.06                     | 0.55              |
| 39:RT:107:ASP:O    | 39:RT:111:ARG:NH1  | 2.39                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:XB:187:LEU:HD22 | 2:XB:201:ILE:O     | 2.07                     | 0.55              |
| 8:XH:102:ARG:HH11 | 8:XH:105:ARG:CZ    | 2.19                     | 0.55              |
| 13:XM:80:ARG:O    | 13:XM:84:ILE:HB    | 2.06                     | 0.55              |
| 13:XM:117:VAL:O   | 13:XM:118:ALA:C    | 2.51                     | 0.55              |
| 16:XP:21:VAL:O    | 16:XP:33:ILE:N     | 2.39                     | 0.55              |
| 16:XP:43:LYS:HA   | 16:XP:48:TRP:CB    | 2.37                     | 0.55              |
| 25:YA:74:A:H4'    | 25:YA:75:G:O5'     | 2.07                     | 0.55              |
| 25:YA:86:C:H4'    | 25:YA:104:U:H1'    | 1.89                     | 0.55              |
| 27:YD:31:LYS:O    | 27:YD:35:LYS:O     | 2.24                     | 0.55              |
| 29:YF:32:LEU:HD12 | 29:YF:36:VAL:HG23  | 1.89                     | 0.55              |
| 40:YU:27:LEU:O    | 40:YU:29:SER:N     | 2.40                     | 0.55              |
| 42:YW:88:ARG:HB3  | 42:YW:92:ARG:HB3   | 1.89                     | 0.55              |
| 43:YX:65:ARG:HD3  | 43:YX:65:ARG:H     | 1.70                     | 0.55              |
| 44:YY:95:LYS:HA   | 44:YY:101:LYS:H    | 1.72                     | 0.55              |
| 44:YY:95:LYS:CB   | 44:YY:100:ALA:HA   | 2.13                     | 0.55              |
| 47:Y1:83:GLU:OE1  | 47:Y1:85:LEU:HD23  | 2.07                     | 0.55              |
| 50:Y4:51:ASP:OD1  | 50:Y4:51:ASP:O     | 2.25                     | 0.55              |
| 1:QA:384:G:H2'    | 1:QA:385:C:C6      | 2.42                     | 0.54              |
| 1:QA:954:G:H21    | 1:QA:1227:A:H62    | 1.53                     | 0.54              |
| 2:QB:80:ILE:CG2   | 2:QB:212:GLN:HA    | 2.35                     | 0.54              |
| 2:QB:214:ILE:HA   | 2:QB:217:ARG:NH2   | 2.22                     | 0.54              |
| 7:QG:50:ILE:CB    | 7:QG:58:PRO:HB3    | 2.37                     | 0.54              |
| 9:QI:66:ARG:HG2   | 9:QI:66:ARG:NH1    | 2.22                     | 0.54              |
| 9:QI:70:LYS:O     | 9:QI:74:ILE:HG13   | 2.07                     | 0.54              |
| 14:QN:24:CYS:SG   | 14:QN:39:LEU:CA    | 2.94                     | 0.54              |
| 16:QP:21:VAL:O    | 16:QP:33:ILE:N     | 2.39                     | 0.54              |
| 17:QQ:33:GLY:O    | 17:QQ:34:LYS:O     | 2.25                     | 0.54              |
| 25:RA:1799:G:H4'  | 25:RA:1800:C:O5'   | 2.07                     | 0.54              |
| 27:RD:25:THR:HG21 | 27:RD:81:ALA:CB    | 2.38                     | 0.54              |
| 27:RD:43:ARG:CB   | 27:RD:54:ARG:HB2   | 2.37                     | 0.54              |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:HD3   | 1.89                     | 0.54              |
| 31:RH:12:PRO:O    | 31:RH:13:LYS:HB2   | 2.07                     | 0.54              |
| 34:RO:53:LYS:HD2  | 34:RO:56:ASP:OD1   | 2.07                     | 0.54              |
| 35:RP:49:ARG:NE   | 54:R8:59:LYS:HG2   | 2.22                     | 0.54              |
| 35:RP:59:LEU:O    | 35:RP:59:LEU:HD23  | 2.06                     | 0.54              |
| 35:RP:84:ASN:ND2  | 35:RP:115:LEU:HD12 | 2.22                     | 0.54              |
| 38:RS:74:ALA:HB1  | 38:RS:107:GLU:HB3  | 1.89                     | 0.54              |
| 40:RU:6:THR:O     | 40:RU:9:VAL:HG23   | 2.07                     | 0.54              |
| 41:RV:49:THR:CB   | 41:RV:50:PRO:CD    | 2.83                     | 0.54              |
| 42:RW:25:ARG:HH11 | 42:RW:25:ARG:CB    | 2.20                     | 0.54              |
| 43:RX:5:TYR:HE2   | 48:R2:30:ARG:HH11  | 1.55                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:R2:47:ASN:ND2   | 48:R2:47:ASN:N     | 2.54                     | 0.54              |
| 2:XB:16:HIS:CE1    | 2:XB:209:ARG:HH21  | 2.25                     | 0.54              |
| 6:XF:89:MET:HE1    | 18:XR:76:LEU:CD2   | 2.36                     | 0.54              |
| 8:XH:119:LEU:HD12  | 8:XH:124:ALA:HA    | 1.87                     | 0.54              |
| 9:XI:40:LEU:HD11   | 9:XI:70:LYS:CG     | 2.37                     | 0.54              |
| 9:XI:70:LYS:O      | 9:XI:74:ILE:HG13   | 2.07                     | 0.54              |
| 9:XI:105:ASP:C     | 9:XI:107:ARG:H     | 2.14                     | 0.54              |
| 9:XI:114:TYR:O     | 9:XI:114:TYR:CD2   | 2.58                     | 0.54              |
| 19:XS:15:LEU:CD2   | 19:XS:15:LEU:H     | 2.21                     | 0.54              |
| 20:XT:10:LEU:HG    | 20:XT:12:ALA:H     | 1.70                     | 0.54              |
| 25:YA:2086:U:H2'   | 25:YA:2087:G:C8    | 2.42                     | 0.54              |
| 27:YD:65:ILE:HD13  | 27:YD:65:ILE:C     | 2.32                     | 0.54              |
| 27:YD:155:LEU:HD23 | 27:YD:177:LEU:CD2  | 2.36                     | 0.54              |
| 28:YE:54:GLN:NE2   | 28:YE:54:GLN:N     | 2.56                     | 0.54              |
| 37:YR:12:ARG:HH11  | 37:YR:12:ARG:HG3   | 1.71                     | 0.54              |
| 38:YS:36:TYR:HD2   | 38:YS:52:SER:CB    | 2.19                     | 0.54              |
| 41:YV:49:THR:CB    | 41:YV:50:PRO:CD    | 2.83                     | 0.54              |
| 54:Y8:30:ARG:O     | 54:Y8:31:HIS:CB    | 2.55                     | 0.54              |
| 2:QB:41:ILE:HD12   | 2:QB:41:ILE:N      | 2.21                     | 0.54              |
| 3:QC:181:ASN:HD21  | 3:QC:204:LEU:CD1   | 2.12                     | 0.54              |
| 6:QF:91:VAL:CG1    | 18:QR:72:ARG:HH12  | 2.18                     | 0.54              |
| 10:QJ:19:SER:O     | 10:QJ:23:ILE:HG13  | 2.07                     | 0.54              |
| 11:QK:125:PHE:HD1  | 11:QK:125:PHE:N    | 2.05                     | 0.54              |
| 12:QL:28:LYS:O     | 12:QL:29:GLY:C     | 2.50                     | 0.54              |
| 13:QM:121:LYS:HE2  | 13:QM:121:LYS:N    | 2.22                     | 0.54              |
| 21:QU:21:TYR:O     | 21:QU:22:ARG:HB2   | 2.05                     | 0.54              |
| 25:RA:336:C:HO2'   | 44:RY:35:TYR:HH    | 1.56                     | 0.54              |
| 25:RA:593:G:O3'    | 54:R8:61:LEU:HD22  | 2.08                     | 0.54              |
| 25:RA:1543:A:HO2'  | 25:RA:1544:C:H3'   | 1.72                     | 0.54              |
| 29:RF:62:ARG:HB3   | 29:RF:62:ARG:NH1   | 2.22                     | 0.54              |
| 29:RF:197:ASP:O    | 29:RF:199:TRP:N    | 2.38                     | 0.54              |
| 30:RG:83:ARG:HB2   | 30:RG:86:MET:HE3   | 1.89                     | 0.54              |
| 30:RG:116:ASP:O    | 30:RG:117:PHE:CB   | 2.50                     | 0.54              |
| 31:RH:8:PRO:O      | 31:RH:9:ILE:HG23   | 2.08                     | 0.54              |
| 33:RN:44:PRO:HG2   | 33:RN:45:ASN:H     | 1.71                     | 0.54              |
| 35:RP:24:GLY:O     | 35:RP:25:SER:HB3   | 2.07                     | 0.54              |
| 38:RS:107:GLU:N    | 38:RS:110:LEU:HD11 | 2.22                     | 0.54              |
| 40:RU:58:ARG:NH1   | 40:RU:93:LYS:HE2   | 2.22                     | 0.54              |
| 42:RW:70:TYR:CD2   | 42:RW:70:TYR:N     | 2.75                     | 0.54              |
| 45:RZ:110:GLY:HA2  | 45:RZ:111:VAL:O    | 2.07                     | 0.54              |
| 45:RZ:150:LEU:HD23 | 45:RZ:171:ILE:HG13 | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:R1:91:LYS:HA    | 47:R1:91:LYS:CE    | 2.37                     | 0.54              |
| 49:R3:8:LEU:HD22   | 49:R3:31:LEU:CD2   | 2.37                     | 0.54              |
| 53:R7:48:LYS:HG2   | 53:R7:49:ARG:N     | 2.19                     | 0.54              |
| 3:XC:43:LEU:O      | 3:XC:47:LEU:HB3    | 2.07                     | 0.54              |
| 4:XD:19:LEU:N      | 4:XD:19:LEU:HD23   | 2.23                     | 0.54              |
| 9:XI:9:ARG:HB2     | 9:XI:14:VAL:HG22   | 1.88                     | 0.54              |
| 9:XI:127:LYS:HE2   | 22:XV:34:C:OP2     | 2.06                     | 0.54              |
| 12:XL:62:SER:C     | 12:XL:64:TYR:H     | 2.14                     | 0.54              |
| 13:XM:121:LYS:HE2  | 13:XM:121:LYS:N    | 2.23                     | 0.54              |
| 16:XP:28:ARG:HG2   | 16:XP:28:ARG:NH1   | 2.22                     | 0.54              |
| 25:YA:76:C:O2'     | 48:Y2:62:THR:HG21  | 2.07                     | 0.54              |
| 25:YA:1203:G:H3'   | 25:YA:1204:A:H5''  | 1.88                     | 0.54              |
| 28:YE:176:ILE:HG22 | 28:YE:179:GLU:H    | 1.72                     | 0.54              |
| 30:YG:41:GLN:HB3   | 30:YG:43:LEU:HD13  | 1.87                     | 0.54              |
| 31:YH:26:VAL:CG1   | 31:YH:27:LYS:N     | 2.63                     | 0.54              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:CB   | 2.37                     | 0.54              |
| 34:YO:53:LYS:HD2   | 34:YO:56:ASP:OD1   | 2.08                     | 0.54              |
| 39:YT:98:LYS:HB3   | 39:YT:100:TYR:CE1  | 2.43                     | 0.54              |
| 40:YU:58:ARG:NH1   | 40:YU:93:LYS:HE2   | 2.22                     | 0.54              |
| 40:YU:95:LEU:HD12  | 41:YV:11:GLN:HE21  | 1.72                     | 0.54              |
| 42:YW:9:TYR:H      | 42:YW:102:HIS:CE1  | 2.25                     | 0.54              |
| 44:YY:2:ARG:HG2    | 44:YY:2:ARG:NH1    | 2.22                     | 0.54              |
| 48:Y2:31:GLU:HB2   | 48:Y2:53:LEU:HD11  | 1.89                     | 0.54              |
| 1:QA:437:U:H2'     | 1:QA:438:G:O4'     | 2.08                     | 0.54              |
| 2:QB:68:ILE:HD12   | 2:QB:68:ILE:N      | 2.21                     | 0.54              |
| 3:QC:43:LEU:O      | 3:QC:47:LEU:HB3    | 2.08                     | 0.54              |
| 3:QC:134:ILE:HG21  | 3:QC:168:ALA:HB3   | 1.89                     | 0.54              |
| 6:QF:52:ILE:O      | 6:QF:53:ALA:HB3    | 2.07                     | 0.54              |
| 8:QH:51:VAL:HG11   | 8:QH:60:ARG:CG     | 2.37                     | 0.54              |
| 16:QP:43:LYS:HA    | 16:QP:48:TRP:CB    | 2.37                     | 0.54              |
| 20:QT:43:LEU:HA    | 20:QT:46:GLU:HB3   | 1.88                     | 0.54              |
| 25:RA:987:G:O2'    | 25:RA:1000:A:N3    | 2.38                     | 0.54              |
| 25:RA:2311:A:C1'   | 30:RG:82:LEU:HD11  | 2.37                     | 0.54              |
| 27:RD:72:LYS:O     | 27:RD:73:VAL:C     | 2.50                     | 0.54              |
| 42:RW:80:PRO:O     | 42:RW:100:THR:CG2  | 2.55                     | 0.54              |
| 44:RY:47:LYS:C     | 44:RY:49:VAL:H     | 2.16                     | 0.54              |
| 45:RZ:163:LEU:H    | 45:RZ:163:LEU:HD12 | 1.71                     | 0.54              |
| 2:XB:134:GLU:O     | 2:XB:138:LEU:HD12  | 2.07                     | 0.54              |
| 8:XH:97:VAL:CG1    | 8:XH:98:LYS:N      | 2.70                     | 0.54              |
| 9:XI:66:ARG:HG2    | 9:XI:66:ARG:NH1    | 2.21                     | 0.54              |
| 10:XJ:32:ALA:O     | 10:XJ:33:GLN:O     | 2.25                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:XK:50:TYR:HH    | 11:XK:59:TYR:HE2   | 1.55                     | 0.54              |
| 12:XL:6:THR:OG1    | 12:XL:9:GLN:HG3    | 2.08                     | 0.54              |
| 13:XM:82:MET:O     | 13:XM:83:ASP:C     | 2.49                     | 0.54              |
| 14:XN:13:THR:N     | 14:XN:14:PRO:HD2   | 2.21                     | 0.54              |
| 14:XN:15:LYS:O     | 14:XN:16:PHE:O     | 2.24                     | 0.54              |
| 25:YA:463:G:N2     | 25:YA:466:A:OP2    | 2.36                     | 0.54              |
| 25:YA:1021:A:H3'   | 25:YA:1021:A:C8    | 2.42                     | 0.54              |
| 25:YA:1309:G:P     | 53:Y7:9:ARG:HD3    | 2.47                     | 0.54              |
| 25:YA:1416:G:H2'   | 25:YA:1417:C:C6    | 2.42                     | 0.54              |
| 25:YA:1693:U:H1'   | 27:YD:14:ARG:NH2   | 2.21                     | 0.54              |
| 25:YA:2011:U:OP2   | 42:YW:16:LYS:NZ    | 2.39                     | 0.54              |
| 31:YH:8:PRO:O      | 31:YH:9:ILE:HG23   | 2.08                     | 0.54              |
| 31:YH:126:PRO:HD2  | 31:YH:127:GLU:H    | 1.72                     | 0.54              |
| 35:YP:104:GLY:C    | 35:YP:105:LEU:HD12 | 2.31                     | 0.54              |
| 35:YP:106:LEU:O    | 35:YP:107:LYS:HD3  | 2.07                     | 0.54              |
| 35:YP:114:ILE:HD11 | 35:YP:130:PHE:HE1  | 1.70                     | 0.54              |
| 41:YV:27:ALA:O     | 41:YV:28:GLU:O     | 2.24                     | 0.54              |
| 41:YV:52:VAL:O     | 41:YV:54:GLY:N     | 2.39                     | 0.54              |
| 47:Y1:92:LYS:O     | 47:Y1:94:LEU:N     | 2.41                     | 0.54              |
| 51:Y5:55:ARG:HD3   | 51:Y5:56:LYS:H     | 1.73                     | 0.54              |
| 2:QB:83:MET:O      | 2:QB:85:ALA:N      | 2.41                     | 0.54              |
| 4:QD:19:LEU:N      | 4:QD:19:LEU:HD23   | 2.23                     | 0.54              |
| 7:QG:62:PHE:O      | 7:QG:66:VAL:HG23   | 2.06                     | 0.54              |
| 16:QP:28:ARG:HG2   | 16:QP:28:ARG:NH1   | 2.22                     | 0.54              |
| 25:RA:2009:G:OP1   | 42:RW:41:LYS:HE2   | 2.07                     | 0.54              |
| 25:RA:2692:C:O2    | 25:RA:2847:U:O2'   | 2.25                     | 0.54              |
| 28:RE:61:ARG:O     | 28:RE:62:PRO:C     | 2.51                     | 0.54              |
| 28:RE:186:GLY:O    | 28:RE:188:VAL:N    | 2.40                     | 0.54              |
| 29:RF:67:GLN:O     | 29:RF:68:LYS:CB    | 2.39                     | 0.54              |
| 29:RF:197:ASP:O    | 29:RF:198:ALA:HB3  | 2.06                     | 0.54              |
| 31:RH:86:GLU:HG3   | 31:RH:165:ALA:CB   | 2.38                     | 0.54              |
| 32:RI:88:ILE:HG12  | 32:RI:122:GLU:H    | 1.71                     | 0.54              |
| 36:RQ:21:THR:O     | 36:RQ:22:LYS:O     | 2.25                     | 0.54              |
| 39:RT:3:ARG:HG3    | 39:RT:7:ILE:CG1    | 2.36                     | 0.54              |
| 39:RT:16:ARG:HG2   | 39:RT:18:ASP:OD1   | 2.07                     | 0.54              |
| 39:RT:29:ARG:HB2   | 39:RT:29:ARG:HH11  | 1.72                     | 0.54              |
| 41:RV:22:VAL:CG1   | 41:RV:23:GLU:N     | 2.71                     | 0.54              |
| 44:RY:47:LYS:O     | 44:RY:49:VAL:HG23  | 2.07                     | 0.54              |
| 47:R1:83:GLU:CG    | 47:R1:84:GLY:N     | 2.71                     | 0.54              |
| 50:R4:37:SER:HB3   | 50:R4:42:PHE:CD1   | 2.43                     | 0.54              |
| 1:XA:1226:C:OP2    | 13:XM:103:THR:OG1  | 2.18                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:XD:153:ARG:NH1  | 4:XD:181:MET:CG   | 2.71                     | 0.54              |
| 5:XE:10:MET:HE2   | 5:XE:13:ILE:HD13  | 1.89                     | 0.54              |
| 8:XH:77:GLU:HG2   | 8:XH:78:GLN:N     | 2.22                     | 0.54              |
| 13:XM:73:GLU:O    | 13:XM:77:ASN:N    | 2.33                     | 0.54              |
| 13:XM:108:ARG:O   | 13:XM:109:THR:C   | 2.50                     | 0.54              |
| 25:YA:323:G:H2'   | 29:YF:169:ASN:OD1 | 2.07                     | 0.54              |
| 25:YA:709:U:H2'   | 25:YA:710:G:C8    | 2.42                     | 0.54              |
| 25:YA:2667:C:H1'  | 31:YH:109:PHE:HD2 | 1.73                     | 0.54              |
| 32:YI:68:LEU:HA   | 32:YI:71:ILE:HG22 | 1.90                     | 0.54              |
| 37:YR:28:LEU:HD13 | 37:YR:28:LEU:O    | 2.08                     | 0.54              |
| 42:YW:80:PRO:O    | 42:YW:100:THR:CG2 | 2.55                     | 0.54              |
| 50:Y4:47:GLN:O    | 50:Y4:48:ARG:HB2  | 2.07                     | 0.54              |
| 50:Y4:63:TYR:C    | 50:Y4:65:ASP:N    | 2.61                     | 0.54              |
| 1:QA:1368:G:OP1   | 9:QI:111:ARG:NH2  | 2.41                     | 0.54              |
| 4:QD:13:ARG:HD2   | 4:QD:40:PRO:HD3   | 1.89                     | 0.54              |
| 11:QK:62:GLN:O    | 11:QK:63:LEU:C    | 2.51                     | 0.54              |
| 18:QR:39:VAL:HA   | 18:QR:42:ARG:NH1  | 2.23                     | 0.54              |
| 25:RA:27:G:H22    | 25:RA:512:G:H2'   | 1.71                     | 0.54              |
| 25:RA:1688:U:H1'  | 25:RA:1701:A:C6   | 2.42                     | 0.54              |
| 27:RD:233:HIS:CD2 | 27:RD:233:HIS:N   | 2.75                     | 0.54              |
| 35:RP:65:ARG:HH21 | 54:R8:15:LYS:HB2  | 1.72                     | 0.54              |
| 36:RQ:39:PRO:HB3  | 36:RQ:99:PRO:HD3  | 1.90                     | 0.54              |
| 39:RT:123:GLN:O   | 39:RT:125:ARG:N   | 2.40                     | 0.54              |
| 42:RW:9:TYR:H     | 42:RW:102:HIS:CE1 | 2.26                     | 0.54              |
| 42:RW:38:TYR:OH   | 51:R5:47:PRO:HG3  | 2.08                     | 0.54              |
| 44:RY:61:ILE:HG23 | 44:RY:62:GLU:H    | 1.71                     | 0.54              |
| 44:RY:95:LYS:HD3  | 44:RY:95:LYS:N    | 2.23                     | 0.54              |
| 49:R3:35:ARG:HB3  | 49:R3:37:LEU:CD2  | 2.37                     | 0.54              |
| 54:R8:32:LEU:O    | 54:R8:36:LYS:HE3  | 2.07                     | 0.54              |
| 1:XA:651:C:N4     | 1:XA:753:A:OP2    | 2.33                     | 0.54              |
| 14:XN:6:LEU:CD2   | 14:XN:23:ARG:NH2  | 2.70                     | 0.54              |
| 15:XO:21:ASP:OD1  | 15:XO:24:SER:HB2  | 2.07                     | 0.54              |
| 15:XO:32:LEU:O    | 15:XO:33:THR:C    | 2.51                     | 0.54              |
| 16:XP:48:TRP:O    | 16:XP:49:LEU:HB2  | 2.06                     | 0.54              |
| 25:YA:995:C:N4    | 33:YN:2:LYS:HG3   | 2.23                     | 0.54              |
| 25:YA:1085:A:O2'  | 25:YA:1086:A:OP1  | 2.24                     | 0.54              |
| 25:YA:1317:A:H2'  | 25:YA:1318:C:C6   | 2.43                     | 0.54              |
| 25:YA:2336:A:H61  | 46:Y0:43:THR:HG21 | 1.72                     | 0.54              |
| 26:YB:80:U:H2'    | 26:YB:81:G:H21    | 1.73                     | 0.54              |
| 27:YD:72:LYS:O    | 27:YD:73:VAL:C    | 2.51                     | 0.54              |
| 28:YE:14:ILE:HG23 | 28:YE:15:PHE:N    | 2.23                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:127:GLU:O    | 29:YF:129:PHE:N    | 2.39                     | 0.54              |
| 29:YF:129:PHE:O    | 29:YF:130:ALA:CB   | 2.55                     | 0.54              |
| 30:YG:3:LEU:HD12   | 30:YG:4:ASP:N      | 2.19                     | 0.54              |
| 33:YN:42:TRP:CD1   | 40:YU:63:VAL:HG11  | 2.43                     | 0.54              |
| 35:YP:24:GLY:O     | 35:YP:25:SER:HB3   | 2.06                     | 0.54              |
| 35:YP:65:ARG:HH21  | 54:Y8:15:LYS:HB2   | 1.72                     | 0.54              |
| 38:YS:111:GLU:HA   | 38:YS:111:GLU:OE1  | 2.07                     | 0.54              |
| 44:YY:95:LYS:HB2   | 44:YY:95:LYS:NZ    | 2.21                     | 0.54              |
| 44:YY:97:ARG:NH2   | 44:YY:98:VAL:CB    | 2.65                     | 0.54              |
| 47:Y1:53:VAL:HG12  | 47:Y1:54:ALA:N     | 2.21                     | 0.54              |
| 51:Y5:44:THR:O     | 51:Y5:46:CYS:N     | 2.40                     | 0.54              |
| 54:Y8:56:GLU:O     | 54:Y8:57:ARG:C     | 2.50                     | 0.54              |
| 1:QA:1397:C:O2'    | 24:QX:8:A:N6       | 2.41                     | 0.54              |
| 8:QH:97:VAL:CG1    | 8:QH:98:LYS:N      | 2.70                     | 0.54              |
| 8:QH:101:PRO:HG2   | 8:QH:133:LEU:HD11  | 1.89                     | 0.54              |
| 13:QM:108:ARG:O    | 13:QM:109:THR:C    | 2.50                     | 0.54              |
| 15:QO:21:ASP:OD1   | 15:QO:24:SER:HB2   | 2.07                     | 0.54              |
| 15:QO:87:ILE:CG2   | 15:QO:88:ARG:H     | 2.00                     | 0.54              |
| 16:QP:3:LYS:O      | 16:QP:21:VAL:HA    | 2.08                     | 0.54              |
| 25:RA:1178:C:H2'   | 25:RA:1179:C:C6    | 2.42                     | 0.54              |
| 25:RA:2790:A:H2'   | 25:RA:2791:C:H5''  | 1.90                     | 0.54              |
| 27:RD:227:ASN:HB3  | 27:RD:228:PRO:CD   | 2.30                     | 0.54              |
| 30:RG:111:LEU:HB2  | 50:R4:38:LYS:HZ3   | 1.72                     | 0.54              |
| 30:RG:139:LEU:HD22 | 30:RG:146:TYR:HD1  | 1.73                     | 0.54              |
| 32:RI:4:ILE:HG12   | 32:RI:18:VAL:HG22  | 1.89                     | 0.54              |
| 32:RI:94:ALA:H     | 32:RI:116:LEU:HD13 | 1.73                     | 0.54              |
| 48:R2:31:GLU:HB2   | 48:R2:53:LEU:HD11  | 1.89                     | 0.54              |
| 51:R5:20:ARG:C     | 51:R5:22:HIS:H     | 2.14                     | 0.54              |
| 52:R6:12:GLU:HG2   | 52:R6:52:VAL:O     | 2.07                     | 0.54              |
| 1:XA:1288:A:N3     | 1:XA:1352:C:O2'    | 2.32                     | 0.54              |
| 3:XC:109:PRO:O     | 3:XC:115:LEU:HD12  | 2.08                     | 0.54              |
| 3:XC:195:VAL:CG1   | 3:XC:196:LEU:N     | 2.71                     | 0.54              |
| 4:XD:196:LEU:C     | 4:XD:198:VAL:N     | 2.65                     | 0.54              |
| 14:XN:22:THR:HB    | 14:XN:33:VAL:HG11  | 1.88                     | 0.54              |
| 27:YD:118:VAL:HG22 | 27:YD:119:ALA:H    | 1.72                     | 0.54              |
| 27:YD:124:PRO:HB2  | 27:YD:126:GLN:NE2  | 2.22                     | 0.54              |
| 27:YD:158:ALA:HB3  | 27:YD:161:THR:HG21 | 1.90                     | 0.54              |
| 27:YD:206:LEU:O    | 27:YD:211:ARG:NH1  | 2.38                     | 0.54              |
| 28:YE:25:VAL:HG11  | 39:YT:11:GLU:HG2   | 1.90                     | 0.54              |
| 30:YG:7:LEU:HD12   | 30:YG:104:GLU:HA   | 1.88                     | 0.54              |
| 30:YG:81:LYS:O     | 30:YG:82:LEU:CB    | 2.56                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:YN:68:GLU:HG2   | 33:YN:88:GLU:CD   | 2.33                     | 0.54              |
| 35:YP:140:ALA:O    | 35:YP:141:ALA:HB2 | 2.08                     | 0.54              |
| 37:YR:18:LEU:HD13  | 37:YR:18:LEU:C    | 2.33                     | 0.54              |
| 44:YY:47:LYS:O     | 44:YY:49:VAL:HG23 | 2.08                     | 0.54              |
| 54:Y8:32:LEU:O     | 54:Y8:36:LYS:HE3  | 2.07                     | 0.54              |
| 1:QA:1014:A:H4'    | 19:QS:14:HIS:HE2  | 1.73                     | 0.54              |
| 3:QC:109:PRO:O     | 3:QC:115:LEU:HD12 | 2.08                     | 0.54              |
| 6:QF:92:LYS:HB2    | 6:QF:92:LYS:NZ    | 2.22                     | 0.54              |
| 10:QJ:101:VAL:HG22 | 10:QJ:101:VAL:O   | 2.07                     | 0.54              |
| 12:QL:6:THR:O      | 12:QL:7:ILE:C     | 2.51                     | 0.54              |
| 13:QM:34:LEU:CD1   | 13:QM:41:PRO:HG3  | 2.38                     | 0.54              |
| 25:RA:486:C:H4'    | 42:RW:60:ASN:OD1  | 2.07                     | 0.54              |
| 25:RA:1007:C:OP1   | 33:RN:35:ARG:NH1  | 2.41                     | 0.54              |
| 27:RD:183:ARG:HG2  | 27:RD:183:ARG:NH1 | 2.11                     | 0.54              |
| 28:RE:176:ILE:HG22 | 28:RE:179:GLU:H   | 1.71                     | 0.54              |
| 35:RP:125:VAL:O    | 35:RP:145:PRO:HD2 | 2.08                     | 0.54              |
| 36:RQ:80:GLU:OE1   | 46:R0:7:LEU:HB3   | 2.08                     | 0.54              |
| 37:RR:45:ARG:HA    | 37:RR:95:THR:HG21 | 1.87                     | 0.54              |
| 38:RS:67:ARG:NH1   | 38:RS:67:ARG:CB   | 2.64                     | 0.54              |
| 41:RV:91:TYR:C     | 41:RV:91:TYR:HD1  | 2.16                     | 0.54              |
| 43:RX:18:TYR:C     | 43:RX:20:GLY:N    | 2.64                     | 0.54              |
| 51:R5:55:ARG:HD3   | 51:R5:56:LYS:H    | 1.73                     | 0.54              |
| 1:XA:718:G:H5'     | 11:XK:117:ASN:OD1 | 2.07                     | 0.54              |
| 7:XG:46:ALA:HB2    | 7:XG:117:ALA:HB1  | 1.88                     | 0.54              |
| 7:XG:102:ARG:O     | 7:XG:106:GLN:HG3  | 2.08                     | 0.54              |
| 8:XH:101:PRO:HG2   | 8:XH:133:LEU:HD11 | 1.89                     | 0.54              |
| 16:XP:3:LYS:O      | 16:XP:21:VAL:HA   | 2.08                     | 0.54              |
| 18:XR:29:PHE:CD2   | 18:XR:29:PHE:N    | 2.76                     | 0.54              |
| 18:XR:51:LEU:HD22  | 18:XR:55:ARG:HD2  | 1.89                     | 0.54              |
| 25:YA:1036:G:OP1   | 31:YH:59:ARG:HB2  | 2.08                     | 0.54              |
| 25:YA:1812:A:O2'   | 27:YD:45:ASN:HB2  | 2.07                     | 0.54              |
| 27:YD:183:ARG:HG2  | 27:YD:183:ARG:NH1 | 2.12                     | 0.54              |
| 27:YD:211:ARG:HD2  | 27:YD:214:TRP:CZ3 | 2.43                     | 0.54              |
| 29:YF:62:ARG:HB3   | 29:YF:62:ARG:NH1  | 2.22                     | 0.54              |
| 31:YH:153:LYS:CE   | 31:YH:153:LYS:HA  | 2.38                     | 0.54              |
| 35:YP:124:LYS:HA   | 35:YP:143:GLY:O   | 2.08                     | 0.54              |
| 36:YQ:39:PRO:HB3   | 36:YQ:99:PRO:HD3  | 1.89                     | 0.54              |
| 40:YU:24:TYR:O     | 40:YU:29:SER:HB3  | 2.08                     | 0.54              |
| 40:YU:86:ALA:HB1   | 40:YU:88:ILE:HD11 | 1.90                     | 0.54              |
| 41:YV:91:TYR:C     | 41:YV:91:TYR:HD1  | 2.16                     | 0.54              |
| 49:Y3:2:PRO:O      | 49:Y3:3:ARG:O     | 2.25                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:Y3:56:VAL:CG1   | 49:Y3:57:GLU:H     | 2.19                     | 0.54              |
| 50:Y4:42:PHE:O     | 50:Y4:43:TYR:C     | 2.51                     | 0.54              |
| 50:Y4:65:ASP:O     | 50:Y4:66:SER:HB3   | 2.07                     | 0.54              |
| 52:Y6:17:LYS:O     | 52:Y6:18:ARG:HB2   | 2.08                     | 0.54              |
| 52:Y6:20:ASN:CG    | 52:Y6:21:TYR:N     | 2.66                     | 0.54              |
| 1:QA:8:A:N6        | 4:QD:205:GLU:O     | 2.40                     | 0.54              |
| 1:QA:243:A:H4'     | 1:QA:244:U:O5'     | 2.07                     | 0.54              |
| 1:QA:939:G:H5''    | 7:QG:102:ARG:NH2   | 2.23                     | 0.54              |
| 1:QA:1152:A:H5''   | 10:QJ:13:HIS:HD2   | 1.73                     | 0.54              |
| 2:QB:16:HIS:CE1    | 2:QB:209:ARG:HH21  | 2.25                     | 0.54              |
| 2:QB:55:PHE:HA     | 2:QB:58:ILE:HB     | 1.88                     | 0.54              |
| 6:QF:78:GLU:OE2    | 6:QF:81:ILE:HD12   | 2.08                     | 0.54              |
| 7:QG:13:GLN:O      | 7:QG:24:THR:HG21   | 2.08                     | 0.54              |
| 19:QS:62:ILE:C     | 19:QS:63:THR:HG22  | 2.32                     | 0.54              |
| 21:QU:6:ARG:O      | 21:QU:8:THR:N      | 2.39                     | 0.54              |
| 22:QV:68:C:H2'     | 22:QV:69:C:C6      | 2.42                     | 0.54              |
| 25:RA:1114:G:H2'   | 25:RA:1115:G:H8    | 1.73                     | 0.54              |
| 27:RD:25:THR:CG2   | 27:RD:81:ALA:HB1   | 2.38                     | 0.54              |
| 28:RE:54:GLN:NE2   | 28:RE:54:GLN:N     | 2.55                     | 0.54              |
| 28:RE:101:ARG:HB3  | 28:RE:201:THR:OG1  | 2.08                     | 0.54              |
| 29:RF:192:LEU:HD21 | 29:RF:194:MET:CE   | 2.35                     | 0.54              |
| 31:RH:26:VAL:CG1   | 31:RH:27:LYS:N     | 2.64                     | 0.54              |
| 31:RH:91:GLY:O     | 31:RH:94:TYR:HB2   | 2.08                     | 0.54              |
| 33:RN:42:TRP:CD1   | 40:RU:63:VAL:HG11  | 2.42                     | 0.54              |
| 34:RO:4:PRO:O      | 34:RO:5:GLN:HB2    | 2.06                     | 0.54              |
| 36:RQ:60:ARG:HH12  | 36:RQ:113:GLN:HE22 | 1.55                     | 0.54              |
| 37:RR:1:MET:O      | 37:RR:2:ARG:HG3    | 2.08                     | 0.54              |
| 39:RT:14:TYR:H     | 39:RT:14:TYR:HD1   | 1.56                     | 0.54              |
| 40:RU:95:LEU:HD12  | 41:RV:11:GLN:HE21  | 1.72                     | 0.54              |
| 44:RY:87:LYS:NZ    | 44:RY:87:LYS:HB2   | 2.23                     | 0.54              |
| 44:RY:91:GLU:HG3   | 44:RY:92:ASN:H     | 1.72                     | 0.54              |
| 47:R1:83:GLU:CD    | 47:R1:85:LEU:H     | 2.15                     | 0.54              |
| 52:R6:17:LYS:O     | 52:R6:18:ARG:HB2   | 2.08                     | 0.54              |
| 1:XA:966:G:O2'     | 9:XI:127:LYS:O     | 2.25                     | 0.54              |
| 3:XC:134:ILE:CD1   | 3:XC:153:VAL:HG21  | 2.35                     | 0.54              |
| 7:XG:12:LEU:HD22   | 7:XG:12:LEU:N      | 2.23                     | 0.54              |
| 7:XG:13:GLN:O      | 7:XG:24:THR:HG21   | 2.08                     | 0.54              |
| 8:XH:20:TYR:HD1    | 8:XH:65:TYR:HD2    | 1.55                     | 0.54              |
| 9:XI:43:ALA:C      | 9:XI:45:ALA:H      | 2.16                     | 0.54              |
| 11:XK:24:SER:HB3   | 11:XK:27:ASN:O     | 2.08                     | 0.54              |
| 12:XL:119:LYS:C    | 12:XL:120:TYR:HD1  | 2.16                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:XM:30:ALA:O    | 13:XM:31:LYS:C     | 2.49                     | 0.54              |
| 27:YD:25:THR:O    | 27:YD:25:THR:HG23  | 2.07                     | 0.54              |
| 27:YD:130:ALA:C   | 27:YD:131:LEU:HD12 | 2.33                     | 0.54              |
| 33:YN:7:LYS:HD3   | 33:YN:9:VAL:CA     | 2.38                     | 0.54              |
| 34:YO:68:GLU:HA   | 34:YO:78:ARG:HB3   | 1.88                     | 0.54              |
| 44:YY:87:LYS:HB2  | 44:YY:87:LYS:NZ    | 2.23                     | 0.54              |
| 55:Y9:1:MET:HB3   | 55:Y9:4:ARG:CZ     | 2.37                     | 0.54              |
| 1:QA:457:C:H42    | 1:QA:475:G:H1      | 1.53                     | 0.54              |
| 1:QA:923:A:N6     | 1:QA:1392:G:O6     | 2.40                     | 0.54              |
| 2:QB:170:GLU:C    | 2:QB:172:ILE:HD12  | 2.33                     | 0.54              |
| 3:QC:53:ALA:HB2   | 3:QC:115:LEU:HD21  | 1.90                     | 0.54              |
| 3:QC:92:ALA:HB2   | 3:QC:99:VAL:CG1    | 2.37                     | 0.54              |
| 4:QD:23:GLY:HA3   | 4:QD:112:VAL:CG2   | 2.38                     | 0.54              |
| 4:QD:79:PHE:CE2   | 4:QD:83:SER:HB2    | 2.43                     | 0.54              |
| 8:QH:102:ARG:NH1  | 8:QH:105:ARG:NH1   | 2.55                     | 0.54              |
| 12:QL:62:SER:C    | 12:QL:64:TYR:H     | 2.15                     | 0.54              |
| 12:QL:83:VAL:CG2  | 12:QL:100:ILE:HG23 | 2.38                     | 0.54              |
| 14:QN:13:THR:N    | 14:QN:14:PRO:HD2   | 2.22                     | 0.54              |
| 25:RA:1039:G:N2   | 25:RA:1116:C:O2    | 2.39                     | 0.54              |
| 25:RA:2335:A:O2'  | 25:RA:2336:A:H2'   | 2.08                     | 0.54              |
| 25:RA:2563:U:H1'  | 25:RA:2566:A:N6    | 2.22                     | 0.54              |
| 27:RD:158:ALA:HB3 | 27:RD:161:THR:HG21 | 1.89                     | 0.54              |
| 27:RD:227:ASN:CB  | 27:RD:228:PRO:HD2  | 2.24                     | 0.54              |
| 28:RE:53:PRO:O    | 28:RE:74:PRO:HA    | 2.07                     | 0.54              |
| 31:RH:86:GLU:CD   | 31:RH:86:GLU:H     | 2.16                     | 0.54              |
| 32:RI:1:MET:HG3   | 32:RI:23:PRO:HB3   | 1.88                     | 0.54              |
| 35:RP:124:LYS:HA  | 35:RP:143:GLY:O    | 2.08                     | 0.54              |
| 38:RS:111:GLU:OE1 | 38:RS:111:GLU:HA   | 2.06                     | 0.54              |
| 41:RV:45:THR:HG22 | 41:RV:45:THR:O     | 2.08                     | 0.54              |
| 44:RY:94:LYS:HE3  | 44:RY:101:LYS:HZ3  | 1.72                     | 0.54              |
| 50:R4:51:ASP:O    | 50:R4:51:ASP:OD1   | 2.25                     | 0.54              |
| 1:XA:521:G:H4'    | 12:XL:73:GLU:HG3   | 1.90                     | 0.54              |
| 1:XA:538:G:OP1    | 12:XL:113:ARG:HD2  | 2.07                     | 0.54              |
| 2:XB:83:MET:O     | 2:XB:85:ALA:N      | 2.41                     | 0.54              |
| 2:XB:102:LEU:HB3  | 2:XB:180:LEU:HD12  | 1.90                     | 0.54              |
| 3:XC:92:ALA:HB2   | 3:XC:99:VAL:CG1    | 2.38                     | 0.54              |
| 6:XF:89:MET:HG2   | 6:XF:89:MET:O      | 2.08                     | 0.54              |
| 7:XG:113:GLU:HB2  | 7:XG:119:ARG:CG    | 2.35                     | 0.54              |
| 7:XG:137:LYS:O    | 7:XG:141:VAL:HG23  | 2.08                     | 0.54              |
| 8:XH:51:VAL:HG11  | 8:XH:60:ARG:CG     | 2.38                     | 0.54              |
| 9:XI:47:LEU:HB3   | 9:XI:50:LEU:HD12   | 1.90                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:XS:62:ILE:C     | 19:XS:63:THR:HG22 | 2.33                     | 0.54              |
| 25:YA:2439:A:C8    | 25:YA:2439:A:H5'  | 2.43                     | 0.54              |
| 25:YA:2705:A:O2'   | 25:YA:2852:G:OP1  | 2.21                     | 0.54              |
| 28:YE:14:ILE:HD11  | 39:YT:14:TYR:CZ   | 2.42                     | 0.54              |
| 28:YE:51:PHE:O     | 28:YE:74:PRO:HB3  | 2.08                     | 0.54              |
| 31:YH:91:GLY:O     | 31:YH:94:TYR:HB2  | 2.08                     | 0.54              |
| 32:YI:27:ARG:HD3   | 47:Y1:71:TYR:HE1  | 1.73                     | 0.54              |
| 34:YO:55:GLY:O     | 34:YO:56:ASP:C    | 2.50                     | 0.54              |
| 37:YR:38:VAL:HG22  | 37:YR:112:ALA:HB2 | 1.90                     | 0.54              |
| 38:YS:13:ARG:O     | 38:YS:13:ARG:HD2  | 2.07                     | 0.54              |
| 39:YT:55:ASN:O     | 39:YT:57:PHE:O    | 2.26                     | 0.54              |
| 47:Y1:80:LEU:C     | 47:Y1:81:LYS:CE   | 2.77                     | 0.54              |
| 52:Y6:12:GLU:HG2   | 52:Y6:52:VAL:O    | 2.07                     | 0.54              |
| 1:QA:191:G:O2'     | 20:QT:101:GLY:O   | 2.26                     | 0.54              |
| 1:QA:662:G:O2'     | 1:QA:836:G:OP1    | 2.26                     | 0.54              |
| 1:QA:939:G:H5''    | 7:QG:102:ARG:HH22 | 1.72                     | 0.54              |
| 1:QA:1065:U:O5'    | 1:QA:1190:G:N2    | 2.41                     | 0.54              |
| 2:QB:170:GLU:HA    | 2:QB:172:ILE:HD12 | 1.90                     | 0.54              |
| 3:QC:195:VAL:CG1   | 3:QC:196:LEU:N    | 2.71                     | 0.54              |
| 7:QG:102:ARG:O     | 7:QG:106:GLN:HG3  | 2.08                     | 0.54              |
| 9:QI:43:ALA:C      | 9:QI:45:ALA:H     | 2.16                     | 0.54              |
| 9:QI:99:LEU:O      | 9:QI:101:PHE:N    | 2.41                     | 0.54              |
| 22:QV:76:A:C2'     | 56:Z6:76:PPU:O    | 2.56                     | 0.54              |
| 25:RA:995:C:N4     | 33:RN:2:LYS:HG3   | 2.23                     | 0.54              |
| 28:RE:51:PHE:O     | 28:RE:74:PRO:HB3  | 2.08                     | 0.54              |
| 29:RF:29:ASN:CB    | 29:RF:112:MET:HE1 | 2.38                     | 0.54              |
| 34:RO:55:GLY:O     | 34:RO:56:ASP:C    | 2.50                     | 0.54              |
| 35:RP:64:LYS:HG3   | 54:R8:25:MET:SD   | 2.48                     | 0.54              |
| 37:RR:53:HIS:HA    | 37:RR:56:LYS:HD3  | 1.90                     | 0.54              |
| 47:R1:83:GLU:OE1   | 47:R1:85:LEU:HD23 | 2.07                     | 0.54              |
| 47:R1:92:LYS:O     | 47:R1:94:LEU:N    | 2.40                     | 0.54              |
| 51:R5:60:VAL:OXT   | 51:R5:60:VAL:CG1  | 2.56                     | 0.54              |
| 1:XA:765:G:N2      | 1:XA:813:U:OP2    | 2.40                     | 0.54              |
| 1:XA:1129:C:H41    | 1:XA:1141:C:H42   | 1.55                     | 0.54              |
| 3:XC:53:ALA:HB2    | 3:XC:115:LEU:HD21 | 1.90                     | 0.54              |
| 9:XI:53:VAL:CB     | 9:XI:95:LYS:HE3   | 2.36                     | 0.54              |
| 9:XI:99:LEU:O      | 9:XI:101:PHE:N    | 2.41                     | 0.54              |
| 10:XJ:61:GLU:HG3   | 14:XN:58:LYS:HE2  | 1.90                     | 0.54              |
| 10:XJ:101:VAL:HG22 | 10:XJ:101:VAL:O   | 2.07                     | 0.54              |
| 12:XL:52:LEU:O     | 12:XL:54:LYS:NZ   | 2.30                     | 0.54              |
| 17:XQ:65:ILE:HD12  | 17:XQ:65:ILE:H    | 1.73                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:XR:39:VAL:HA   | 18:XR:42:ARG:NH1   | 2.23                     | 0.54              |
| 25:YA:1203:G:H5'  | 35:YP:3:LEU:HD12   | 1.90                     | 0.54              |
| 25:YA:1204:A:H1'  | 25:YA:1206:G:C8    | 2.43                     | 0.54              |
| 25:YA:2159:G:H2'  | 25:YA:2160:G:H8    | 1.73                     | 0.54              |
| 28:YE:186:GLY:O   | 28:YE:188:VAL:N    | 2.41                     | 0.54              |
| 29:YF:197:ASP:O   | 29:YF:198:ALA:HB3  | 2.06                     | 0.54              |
| 31:YH:151:ILE:C   | 31:YH:152:ARG:O    | 2.49                     | 0.54              |
| 34:YO:49:ARG:HB3  | 34:YO:49:ARG:NH1   | 2.23                     | 0.54              |
| 34:YO:78:ARG:O    | 39:YT:73:GLU:HG3   | 2.08                     | 0.54              |
| 35:YP:84:ASN:ND2  | 35:YP:115:LEU:HD12 | 2.22                     | 0.54              |
| 35:YP:92:GLU:HA   | 35:YP:123:LEU:CD2  | 2.38                     | 0.54              |
| 41:YV:66:ARG:HH11 | 41:YV:66:ARG:CB    | 2.20                     | 0.54              |
| 43:YX:5:TYR:HE2   | 48:Y2:30:ARG:HH11  | 1.55                     | 0.54              |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HB2   | 1.90                     | 0.54              |
| 1:QA:382:A:H2'    | 1:QA:383:A:C8      | 2.43                     | 0.53              |
| 8:QH:77:GLU:HG2   | 8:QH:78:GLN:N      | 2.22                     | 0.53              |
| 9:QI:105:ASP:C    | 9:QI:107:ARG:H     | 2.15                     | 0.53              |
| 11:QK:24:SER:HB3  | 11:QK:27:ASN:O     | 2.08                     | 0.53              |
| 12:QL:6:THR:OG1   | 12:QL:9:GLN:HG3    | 2.08                     | 0.53              |
| 13:QM:76:ALA:O    | 13:QM:79:LYS:HB3   | 2.09                     | 0.53              |
| 19:QS:5:LEU:HD22  | 50:R4:67:TYR:HE2   | 1.72                     | 0.53              |
| 19:QS:15:LEU:CD2  | 19:QS:15:LEU:H     | 2.21                     | 0.53              |
| 25:RA:155:C:N4    | 25:RA:171:G:H1     | 2.05                     | 0.53              |
| 25:RA:767:U:H2'   | 25:RA:768:G:H8     | 1.72                     | 0.53              |
| 26:RB:55:U:H2'    | 26:RB:56:G:C8      | 2.43                     | 0.53              |
| 31:RH:153:LYS:HA  | 31:RH:153:LYS:CE   | 2.37                     | 0.53              |
| 33:RN:137:LYS:HG3 | 33:RN:138:LEU:N    | 2.23                     | 0.53              |
| 37:RR:18:LEU:HD13 | 37:RR:18:LEU:C     | 2.33                     | 0.53              |
| 37:RR:38:VAL:HG22 | 37:RR:112:ALA:HB2  | 1.90                     | 0.53              |
| 40:RU:24:TYR:O    | 40:RU:29:SER:HB3   | 2.08                     | 0.53              |
| 52:R6:27:LYS:HB2  | 52:R6:27:LYS:HZ2   | 1.71                     | 0.53              |
| 53:R7:10:ARG:NH1  | 53:R7:14:LYS:HE3   | 2.23                     | 0.53              |
| 12:XL:83:VAL:CG2  | 12:XL:100:ILE:HG23 | 2.38                     | 0.53              |
| 15:XO:77:ARG:HA   | 15:XO:80:ALA:CB    | 2.37                     | 0.53              |
| 19:XS:65:ASN:HA   | 50:Y4:55:ARG:HH11  | 1.72                     | 0.53              |
| 27:YD:80:ALA:HB3  | 27:YD:94:LEU:HD13  | 1.88                     | 0.53              |
| 29:YF:147:GLY:O   | 29:YF:148:LEU:HD23 | 2.07                     | 0.53              |
| 31:YH:12:PRO:O    | 31:YH:13:LYS:HB2   | 2.07                     | 0.53              |
| 34:YO:12:ASP:OD1  | 34:YO:85:VAL:HG13  | 2.08                     | 0.53              |
| 37:YR:70:LEU:HD13 | 37:YR:75:LEU:HD11  | 1.88                     | 0.53              |
| 37:YR:91:GLN:HG2  | 37:YR:91:GLN:O     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:YS:74:ALA:HB1  | 38:YS:107:GLU:HB3  | 1.89                     | 0.53              |
| 41:YV:45:THR:HG22 | 41:YV:45:THR:O     | 2.08                     | 0.53              |
| 41:YV:91:TYR:C    | 41:YV:91:TYR:CD1   | 2.87                     | 0.53              |
| 47:Y1:87:PRO:O    | 47:Y1:91:LYS:N     | 2.31                     | 0.53              |
| 47:Y1:91:LYS:HA   | 47:Y1:91:LYS:CE    | 2.37                     | 0.53              |
| 48:Y2:47:ASN:ND2  | 48:Y2:47:ASN:N     | 2.54                     | 0.53              |
| 1:QA:1172:C:H2'   | 1:QA:1173:G:C8     | 2.43                     | 0.53              |
| 5:QE:12:LEU:O     | 5:QE:13:ILE:HD12   | 2.08                     | 0.53              |
| 7:QG:12:LEU:HD22  | 7:QG:12:LEU:N      | 2.23                     | 0.53              |
| 10:QJ:61:GLU:HG3  | 14:QN:58:LYS:HE2   | 1.90                     | 0.53              |
| 12:QL:42:THR:HA   | 12:QL:53:ARG:O     | 2.08                     | 0.53              |
| 12:QL:119:LYS:C   | 12:QL:120:TYR:HD1  | 2.16                     | 0.53              |
| 25:RA:520:G:H2'   | 25:RA:521:G:H8     | 1.72                     | 0.53              |
| 25:RA:969:U:H2'   | 25:RA:970:C:C6     | 2.43                     | 0.53              |
| 25:RA:1288:U:O2'  | 25:RA:1647:G:N2    | 2.41                     | 0.53              |
| 25:RA:1441:G:H2'  | 25:RA:1442:G:H8    | 1.73                     | 0.53              |
| 27:RD:85:ASP:OD2  | 27:RD:88:ARG:HG2   | 2.07                     | 0.53              |
| 27:RD:124:PRO:HB2 | 27:RD:126:GLN:NE2  | 2.22                     | 0.53              |
| 27:RD:211:ARG:HD2 | 27:RD:214:TRP:CZ3  | 2.43                     | 0.53              |
| 28:RE:14:ILE:CG1  | 28:RE:15:PHE:H     | 2.08                     | 0.53              |
| 31:RH:139:GLN:O   | 31:RH:143:GLN:HB2  | 2.09                     | 0.53              |
| 33:RN:109:LYS:HD2 | 33:RN:109:LYS:H    | 1.74                     | 0.53              |
| 34:RO:78:ARG:O    | 39:RT:73:GLU:HG3   | 2.08                     | 0.53              |
| 34:RO:113:LYS:HG2 | 34:RO:117:LEU:CD1  | 2.39                     | 0.53              |
| 35:RP:37:GLY:HA2  | 35:RP:41:ARG:NE    | 2.24                     | 0.53              |
| 35:RP:140:ALA:O   | 35:RP:141:ALA:HB2  | 2.08                     | 0.53              |
| 41:RV:7:THR:CG2   | 41:RV:22:VAL:HG11  | 2.39                     | 0.53              |
| 47:R1:25:LYS:C    | 47:R1:27:GLU:H     | 2.16                     | 0.53              |
| 48:R2:43:GLN:O    | 48:R2:44:LEU:CG    | 2.54                     | 0.53              |
| 52:R6:20:ASN:CG   | 52:R6:21:TYR:N     | 2.66                     | 0.53              |
| 3:XC:134:ILE:HG21 | 3:XC:168:ALA:HB3   | 1.90                     | 0.53              |
| 5:XE:101:ILE:HG12 | 5:XE:101:ILE:O     | 2.08                     | 0.53              |
| 9:XI:28:VAL:HG13  | 9:XI:63:ILE:HG21   | 1.89                     | 0.53              |
| 10:XJ:16:LEU:O    | 10:XJ:20:ALA:HB2   | 2.08                     | 0.53              |
| 27:YD:85:ASP:OD2  | 27:YD:88:ARG:HG2   | 2.07                     | 0.53              |
| 27:YD:198:ASN:C   | 27:YD:198:ASN:HD22 | 2.16                     | 0.53              |
| 28:YE:101:ARG:HB3 | 28:YE:201:THR:OG1  | 2.08                     | 0.53              |
| 35:YP:14:LYS:O    | 35:YP:15:ARG:C     | 2.51                     | 0.53              |
| 39:YT:105:LEU:O   | 39:YT:107:ASP:N    | 2.41                     | 0.53              |
| 40:YU:74:LEU:HD13 | 40:YU:79:PHE:HB2   | 1.89                     | 0.53              |
| 41:YV:41:GLY:HA3  | 41:YV:46:VAL:CG1   | 2.38                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:Y5:16:ARG:NH1   | 51:Y5:17:ASP:OD1  | 2.41                     | 0.53              |
| 52:Y6:11:LEU:CD1   | 52:Y6:51:GLU:HG3  | 2.39                     | 0.53              |
| 53:Y7:10:ARG:NH1   | 53:Y7:14:LYS:HE3  | 2.23                     | 0.53              |
| 1:QA:1113:C:H2'    | 1:QA:1114:C:C6    | 2.44                     | 0.53              |
| 2:QB:24:TRP:CE2    | 2:QB:26:PRO:HD3   | 2.43                     | 0.53              |
| 2:QB:134:GLU:O     | 2:QB:138:LEU:HD12 | 2.07                     | 0.53              |
| 3:QC:51:GLY:O      | 3:QC:70:VAL:HG13  | 2.09                     | 0.53              |
| 6:QF:41:GLU:HG2    | 6:QF:43:LEU:HD11  | 1.89                     | 0.53              |
| 25:RA:263:C:H2'    | 25:RA:264:C:O4'   | 2.07                     | 0.53              |
| 25:RA:996:A:H4'    | 40:RU:92:ARG:HE   | 1.73                     | 0.53              |
| 27:RD:25:THR:O     | 27:RD:25:THR:HG23 | 2.07                     | 0.53              |
| 30:RG:81:LYS:O     | 30:RG:82:LEU:CB   | 2.56                     | 0.53              |
| 34:RO:49:ARG:HB3   | 34:RO:49:ARG:NH1  | 2.23                     | 0.53              |
| 36:RQ:112:GLU:CD   | 36:RQ:112:GLU:H   | 2.17                     | 0.53              |
| 43:RX:53:LYS:NZ    | 43:RX:55:ASN:HD21 | 2.06                     | 0.53              |
| 51:R5:44:THR:O     | 51:R5:46:CYS:N    | 2.41                     | 0.53              |
| 54:R8:58:ILE:O     | 54:R8:61:LEU:HG   | 2.08                     | 0.53              |
| 1:XA:970:C:N4      | 9:XI:128:ARG:OXT  | 2.42                     | 0.53              |
| 2:XB:140:HIS:C     | 2:XB:142:LEU:H    | 2.16                     | 0.53              |
| 4:XD:120:LEU:HD22  | 4:XD:125:HIS:CB   | 2.38                     | 0.53              |
| 7:XG:50:ILE:HG22   | 7:XG:50:ILE:O     | 2.07                     | 0.53              |
| 12:XL:42:THR:HA    | 12:XL:53:ARG:O    | 2.08                     | 0.53              |
| 13:XM:39:ILE:HD11  | 13:XM:56:LEU:HB2  | 1.90                     | 0.53              |
| 17:XQ:11:VAL:HG22  | 17:XQ:20:THR:O    | 2.09                     | 0.53              |
| 25:YA:221:A:H4'    | 25:YA:222:A:O5'   | 2.08                     | 0.53              |
| 25:YA:469:G:O6     | 53:Y7:37:LYS:HE2  | 2.09                     | 0.53              |
| 25:YA:540:G:H5'    | 25:YA:541:C:OP2   | 2.09                     | 0.53              |
| 28:YE:61:ARG:O     | 28:YE:62:PRO:C    | 2.51                     | 0.53              |
| 30:YG:83:ARG:HB2   | 30:YG:86:MET:HE3  | 1.89                     | 0.53              |
| 30:YG:139:LEU:HD22 | 30:YG:146:TYR:HD1 | 1.73                     | 0.53              |
| 35:YP:88:LEU:HD23  | 35:YP:89:ALA:N    | 2.24                     | 0.53              |
| 37:YR:70:LEU:C     | 37:YR:72:ASP:H    | 2.16                     | 0.53              |
| 38:YS:25:ARG:HH12  | 38:YS:42:ASP:CG   | 2.16                     | 0.53              |
| 44:YY:47:LYS:C     | 44:YY:49:VAL:H    | 2.16                     | 0.53              |
| 45:YZ:10:ARG:HH21  | 45:YZ:26:GLY:H    | 1.55                     | 0.53              |
| 54:Y8:63:PRO:O     | 54:Y8:64:TYR:HB2  | 2.07                     | 0.53              |
| 1:QA:103:C:P       | 20:QT:17:ARG:HH21 | 2.31                     | 0.53              |
| 2:QB:187:LEU:HD22  | 2:QB:201:ILE:O    | 2.07                     | 0.53              |
| 3:QC:3:ASN:ND2     | 3:QC:3:ASN:H      | 2.05                     | 0.53              |
| 4:QD:173:TRP:CD1   | 4:QD:174:LEU:HG   | 2.44                     | 0.53              |
| 9:QI:13:ALA:HA     | 9:QI:66:ARG:O     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:QI:28:VAL:HG13  | 9:QI:63:ILE:HG21  | 1.89                     | 0.53              |
| 11:QK:20:TYR:HB2  | 11:QK:31:THR:O    | 2.07                     | 0.53              |
| 17:QQ:5:VAL:O     | 17:QQ:6:LEU:HD23  | 2.09                     | 0.53              |
| 25:RA:666:G:H4'   | 35:RP:49:ARG:NH1  | 2.24                     | 0.53              |
| 25:RA:1012:U:O2   | 33:RN:25:ARG:NH1  | 2.41                     | 0.53              |
| 26:RB:56:G:H5'    | 30:RG:27:ASN:HD21 | 1.72                     | 0.53              |
| 27:RD:206:LEU:O   | 27:RD:211:ARG:NH1 | 2.38                     | 0.53              |
| 29:RF:32:LEU:HD12 | 29:RF:36:VAL:HG23 | 1.89                     | 0.53              |
| 34:RO:14:THR:HG21 | 34:RO:86:ILE:HD13 | 1.90                     | 0.53              |
| 37:RR:3:HIS:C     | 37:RR:5:LYS:H     | 2.17                     | 0.53              |
| 37:RR:70:LEU:C    | 37:RR:72:ASP:H    | 2.16                     | 0.53              |
| 39:RT:135:ALA:C   | 39:RT:137:LYS:H   | 2.16                     | 0.53              |
| 41:RV:66:ARG:HH11 | 41:RV:66:ARG:CB   | 2.20                     | 0.53              |
| 41:RV:91:TYR:C    | 41:RV:91:TYR:CD1  | 2.87                     | 0.53              |
| 49:R3:2:PRO:O     | 49:R3:3:ARG:O     | 2.25                     | 0.53              |
| 54:R8:29:LYS:HB2  | 54:R8:44:LYS:HG2  | 1.90                     | 0.53              |
| 9:XI:13:ALA:HA    | 9:XI:66:ARG:O     | 2.08                     | 0.53              |
| 12:XL:6:THR:O     | 12:XL:7:ILE:C     | 2.51                     | 0.53              |
| 13:XM:87:TYR:C    | 13:XM:89:GLY:N    | 2.64                     | 0.53              |
| 21:XU:14:TRP:CZ3  | 21:XU:15:ARG:HD3  | 2.43                     | 0.53              |
| 25:YA:138:G:N2    | 43:YX:44:GLU:OE2  | 2.28                     | 0.53              |
| 25:YA:994:C:H3'   | 40:YU:54:LYS:HE3  | 1.91                     | 0.53              |
| 25:YA:2264:C:N4   | 46:Y0:15:ASP:OD2  | 2.41                     | 0.53              |
| 25:YA:2314:C:OP1  | 30:YG:91:ARG:NH1  | 2.42                     | 0.53              |
| 27:YD:35:LYS:CG   | 27:YD:64:ILE:H    | 2.15                     | 0.53              |
| 33:YN:12:ARG:NH1  | 33:YN:50:ASP:CG   | 2.67                     | 0.53              |
| 33:YN:137:LYS:HG3 | 33:YN:138:LEU:N   | 2.23                     | 0.53              |
| 41:YV:22:VAL:CG1  | 41:YV:23:GLU:N    | 2.71                     | 0.53              |
| 44:YY:90:LEU:HD22 | 44:YY:90:LEU:H    | 1.73                     | 0.53              |
| 48:Y2:16:LEU:O    | 48:Y2:16:LEU:CG   | 2.49                     | 0.53              |
| 50:Y4:37:SER:HB3  | 50:Y4:42:PHE:CD1  | 2.43                     | 0.53              |
| 1:QA:1023:G:H3'   | 1:QA:1024:G:H5''  | 1.89                     | 0.53              |
| 1:QA:1346:A:H5''  | 9:QI:120:ARG:HH12 | 1.73                     | 0.53              |
| 2:QB:96:ARG:H     | 2:QB:96:ARG:CD    | 2.16                     | 0.53              |
| 2:QB:134:GLU:HB3  | 2:QB:138:LEU:CD1  | 2.39                     | 0.53              |
| 3:QC:173:VAL:HG12 | 3:QC:173:VAL:O    | 2.08                     | 0.53              |
| 9:QI:4:TYR:CE2    | 9:QI:88:TYR:HB2   | 2.44                     | 0.53              |
| 13:QM:3:ARG:HA    | 13:QM:9:ILE:CG2   | 2.22                     | 0.53              |
| 13:QM:39:ILE:HD11 | 13:QM:56:LEU:HB2  | 1.90                     | 0.53              |
| 15:QO:7:GLU:O     | 15:QO:11:VAL:HG23 | 2.09                     | 0.53              |
| 18:QR:58:LEU:HD12 | 18:QR:58:LEU:H    | 1.72                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:686:G:H21   | 25:RA:788:A:H61    | 1.55                     | 0.53              |
| 29:RF:34:TRP:CH2  | 35:RP:8:PRO:HB3    | 2.43                     | 0.53              |
| 29:RF:116:ASP:OD1 | 29:RF:119:ARG:NH2  | 2.41                     | 0.53              |
| 32:RI:92:VAL:HG13 | 32:RI:120:ILE:HG23 | 1.89                     | 0.53              |
| 34:RO:12:ASP:OD1  | 34:RO:85:VAL:HG13  | 2.08                     | 0.53              |
| 37:RR:28:LEU:HD13 | 37:RR:28:LEU:O     | 2.08                     | 0.53              |
| 37:RR:91:GLN:O    | 37:RR:91:GLN:HG2   | 2.08                     | 0.53              |
| 39:RT:98:LYS:HB3  | 39:RT:100:TYR:CE1  | 2.42                     | 0.53              |
| 43:RX:60:ARG:NH1  | 53:R7:47:ARG:HH22  | 2.07                     | 0.53              |
| 44:RY:44:ILE:CG1  | 44:RY:45:VAL:N     | 2.70                     | 0.53              |
| 44:RY:84:ARG:NH1  | 44:RY:97:ARG:HB2   | 2.11                     | 0.53              |
| 44:RY:97:ARG:NH2  | 44:RY:98:VAL:CB    | 2.65                     | 0.53              |
| 51:R5:16:ARG:NH1  | 51:R5:17:ASP:OD1   | 2.41                     | 0.53              |
| 1:XA:345:C:H1'    | 1:XA:346:G:OP2     | 2.08                     | 0.53              |
| 4:XD:172:PRO:HB2  | 4:XD:193:ASP:OD2   | 2.08                     | 0.53              |
| 4:XD:173:TRP:CD1  | 4:XD:174:LEU:HG    | 2.44                     | 0.53              |
| 7:XG:95:ARG:CZ    | 7:XG:99:LEU:HD11   | 2.38                     | 0.53              |
| 13:XM:34:LEU:CD1  | 13:XM:41:PRO:HG3   | 2.38                     | 0.53              |
| 14:XN:40:CYS:SG   | 14:XN:42:ILE:N     | 2.81                     | 0.53              |
| 17:XQ:33:GLY:O    | 17:XQ:34:LYS:O     | 2.26                     | 0.53              |
| 19:XS:5:LEU:CD2   | 50:Y4:67:TYR:CZ    | 2.91                     | 0.53              |
| 19:XS:63:THR:O    | 19:XS:66:MET:HG2   | 2.09                     | 0.53              |
| 20:XT:30:LYS:HE2  | 20:XT:72:LEU:HD12  | 1.91                     | 0.53              |
| 25:YA:2105:C:H2'  | 25:YA:2106:G:C8    | 2.42                     | 0.53              |
| 28:YE:47:VAL:O    | 28:YE:48:GLN:C     | 2.52                     | 0.53              |
| 36:YQ:112:GLU:CD  | 36:YQ:112:GLU:H    | 2.17                     | 0.53              |
| 39:YT:135:ALA:C   | 39:YT:137:LYS:H    | 2.16                     | 0.53              |
| 42:YW:28:SER:HB3  | 42:YW:31:GLU:HB2   | 1.91                     | 0.53              |
| 52:Y6:13:CYS:O    | 52:Y6:14:THR:HB    | 2.08                     | 0.53              |
| 1:QA:196:A:OP1    | 20:QT:68:LYS:NZ    | 2.38                     | 0.53              |
| 1:QA:816:A:OP1    | 1:QA:1526:G:O2'    | 2.24                     | 0.53              |
| 2:QB:87:ARG:HH11  | 2:QB:223:ILE:HD12  | 1.73                     | 0.53              |
| 3:QC:78:GLY:HA3   | 3:QC:83:ARG:CB     | 2.38                     | 0.53              |
| 4:QD:147:ALA:HA   | 4:QD:182:LYS:HA    | 1.91                     | 0.53              |
| 4:QD:153:ARG:NH1  | 4:QD:181:MET:CG    | 2.71                     | 0.53              |
| 4:QD:166:LYS:CG   | 27:YD:134:ARG:HH12 | 2.17                     | 0.53              |
| 4:QD:198:VAL:HG12 | 4:QD:199:ASN:H     | 1.74                     | 0.53              |
| 5:QE:140:ARG:HB2  | 5:QE:140:ARG:NH1   | 2.23                     | 0.53              |
| 7:QG:137:LYS:O    | 7:QG:141:VAL:HG23  | 2.07                     | 0.53              |
| 10:QJ:16:LEU:O    | 10:QJ:20:ALA:HB2   | 2.08                     | 0.53              |
| 15:QO:32:LEU:O    | 15:QO:33:THR:C     | 2.51                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:QP:43:LYS:C    | 16:QP:45:THR:H     | 2.14                     | 0.53              |
| 18:QR:51:LEU:HD22 | 18:QR:55:ARG:HD2   | 1.89                     | 0.53              |
| 25:RA:1952:A:OP1  | 34:RO:44:LYS:NZ    | 2.25                     | 0.53              |
| 29:RF:198:ALA:C   | 29:RF:200:GLU:N    | 2.62                     | 0.53              |
| 32:RI:11:ASN:O    | 32:RI:12:LEU:HB2   | 2.09                     | 0.53              |
| 33:RN:12:ARG:NH1  | 33:RN:50:ASP:CG    | 2.67                     | 0.53              |
| 33:RN:19:GLU:HA   | 33:RN:59:LYS:HB2   | 1.91                     | 0.53              |
| 33:RN:78:TYR:N    | 33:RN:78:TYR:HD1   | 2.07                     | 0.53              |
| 33:RN:95:PRO:O    | 33:RN:96:GLU:C     | 2.51                     | 0.53              |
| 36:RQ:119:ARG:HG2 | 36:RQ:119:ARG:NH1  | 2.20                     | 0.53              |
| 38:RS:10:ARG:O    | 38:RS:14:VAL:HG12  | 2.09                     | 0.53              |
| 39:RT:105:LEU:O   | 39:RT:107:ASP:N    | 2.41                     | 0.53              |
| 43:RX:36:LYS:HA   | 43:RX:39:ILE:HD12  | 1.90                     | 0.53              |
| 50:R4:15:ILE:HD13 | 50:R4:15:ILE:H     | 1.74                     | 0.53              |
| 52:R6:11:LEU:CD1  | 52:R6:51:GLU:HG3   | 2.39                     | 0.53              |
| 1:XA:1062:U:H2'   | 1:XA:1063:C:C6     | 2.43                     | 0.53              |
| 1:XA:1114:C:H1'   | 14:XN:60:SER:HB2   | 1.89                     | 0.53              |
| 1:XA:1256:A:P     | 3:XC:26:LYS:HZ3    | 2.31                     | 0.53              |
| 1:XA:1391:U:H2'   | 1:XA:1392:G:C8     | 2.43                     | 0.53              |
| 2:XB:206:ASP:O    | 2:XB:207:ALA:HB3   | 2.08                     | 0.53              |
| 4:XD:79:PHE:CE2   | 4:XD:83:SER:HB2    | 2.43                     | 0.53              |
| 7:XG:85:TYR:HE1   | 7:XG:154:TYR:HE1   | 1.56                     | 0.53              |
| 14:XN:41:ARG:HE   | 14:XN:42:ILE:CG1   | 2.22                     | 0.53              |
| 19:XS:7:LYS:HG3   | 19:XS:8:GLY:N      | 2.22                     | 0.53              |
| 25:YA:125:G:H5'   | 53:Y7:19:ARG:HD3   | 1.88                     | 0.53              |
| 25:YA:483:A:H5'   | 44:YY:49:VAL:HG13  | 1.90                     | 0.53              |
| 25:YA:784:A:C5    | 27:YD:229:VAL:HG21 | 2.44                     | 0.53              |
| 25:YA:2543:G:H2'  | 25:YA:2544:G:C8    | 2.44                     | 0.53              |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:CB    | 2.38                     | 0.53              |
| 31:YH:40:GLU:O    | 31:YH:41:MET:HB2   | 2.08                     | 0.53              |
| 31:YH:59:ARG:HH11 | 31:YH:59:ARG:CG    | 2.20                     | 0.53              |
| 33:YN:19:GLU:HA   | 33:YN:59:LYS:HB2   | 1.91                     | 0.53              |
| 33:YN:56:ASN:ND2  | 33:YN:125:GLY:C    | 2.66                     | 0.53              |
| 34:YO:2:ILE:HD12  | 34:YO:2:ILE:N      | 2.23                     | 0.53              |
| 35:YP:64:LYS:HG3  | 54:Y8:25:MET:SD    | 2.48                     | 0.53              |
| 37:YR:67:LEU:HD13 | 37:YR:76:VAL:CG2   | 2.27                     | 0.53              |
| 54:Y8:58:ILE:O    | 54:Y8:61:LEU:HG    | 2.08                     | 0.53              |
| 3:QC:87:LEU:C     | 3:QC:89:GLU:N      | 2.65                     | 0.53              |
| 5:QE:101:ILE:O    | 5:QE:101:ILE:HG12  | 2.08                     | 0.53              |
| 17:QQ:11:VAL:HG22 | 17:QQ:20:THR:O     | 2.09                     | 0.53              |
| 26:RB:48:A:H4'    | 38:RS:95:HIS:HD2   | 1.74                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:RN:120:LEU:CD1 | 33:RN:122:VAL:HG23 | 2.39                     | 0.53              |
| 38:RS:25:ARG:HH11 | 38:RS:25:ARG:CB    | 2.22                     | 0.53              |
| 44:RY:95:LYS:HA   | 44:RY:101:LYS:H    | 1.72                     | 0.53              |
| 1:XA:814:A:O2'    | 1:XA:815:A:H3'     | 2.08                     | 0.53              |
| 1:XA:973:G:O4'    | 10:XJ:55:LYS:HG2   | 2.08                     | 0.53              |
| 2:XB:24:TRP:CE2   | 2:XB:26:PRO:HD3    | 2.43                     | 0.53              |
| 3:XC:3:ASN:ND2    | 3:XC:3:ASN:H       | 2.05                     | 0.53              |
| 3:XC:78:GLY:HA3   | 3:XC:83:ARG:CB     | 2.38                     | 0.53              |
| 5:XE:87:SER:HB3   | 5:XE:131:ILE:CD1   | 2.39                     | 0.53              |
| 6:XF:78:GLU:OE2   | 6:XF:81:ILE:HD12   | 2.08                     | 0.53              |
| 13:XM:81:LEU:HD13 | 13:XM:88:ARG:HD2   | 1.91                     | 0.53              |
| 16:XP:40:ASP:C    | 16:XP:42:ARG:H     | 2.17                     | 0.53              |
| 17:XQ:5:VAL:O     | 17:XQ:6:LEU:HD23   | 2.08                     | 0.53              |
| 18:XR:30:ASP:C    | 18:XR:32:ARG:H     | 2.15                     | 0.53              |
| 25:YA:1329:U:H5'' | 25:YA:1330:C:H5    | 1.73                     | 0.53              |
| 25:YA:1903:G:OP1  | 27:YD:241:PRO:HG2  | 2.09                     | 0.53              |
| 25:YA:2134:A:OP2  | 25:YA:2157:G:N2    | 2.42                     | 0.53              |
| 27:YD:25:THR:CG2  | 27:YD:81:ALA:HB1   | 2.38                     | 0.53              |
| 27:YD:77:ALA:HB2  | 27:YD:97:TYR:CG    | 2.44                     | 0.53              |
| 29:YF:116:ASP:OD1 | 29:YF:119:ARG:NH2  | 2.41                     | 0.53              |
| 31:YH:125:VAL:HA  | 31:YH:126:PRO:CB   | 2.29                     | 0.53              |
| 31:YH:128:PRO:CD  | 31:YH:129:THR:N    | 2.71                     | 0.53              |
| 33:YN:22:THR:CG2  | 33:YN:23:LEU:N     | 2.61                     | 0.53              |
| 35:YP:79:ARG:HD3  | 35:YP:110:TYR:CE1  | 2.43                     | 0.53              |
| 36:YQ:76:LYS:O    | 36:YQ:88:GLY:HA3   | 2.09                     | 0.53              |
| 38:YS:10:ARG:O    | 38:YS:14:VAL:HG12  | 2.09                     | 0.53              |
| 41:YV:48:GLY:O    | 41:YV:49:THR:O     | 2.26                     | 0.53              |
| 50:Y4:49:PHE:N    | 50:Y4:49:PHE:CD1   | 2.77                     | 0.53              |
| 6:QF:75:LEU:HD23  | 6:QF:79:LEU:HG     | 1.91                     | 0.53              |
| 9:QI:47:LEU:HB3   | 9:QI:50:LEU:HD12   | 1.90                     | 0.53              |
| 16:QP:4:ILE:HD12  | 16:QP:4:ILE:N      | 2.23                     | 0.53              |
| 19:QS:29:ARG:HD3  | 19:QS:30:LEU:HD13  | 1.91                     | 0.53              |
| 25:RA:784:A:N7    | 27:RD:229:VAL:HG21 | 2.24                     | 0.53              |
| 25:RA:1190:G:H5'  | 35:RP:32:THR:HA    | 1.91                     | 0.53              |
| 27:RD:36:PRO:HA   | 27:RD:62:TYR:O     | 2.09                     | 0.53              |
| 28:RE:14:ILE:HG23 | 28:RE:15:PHE:N     | 2.22                     | 0.53              |
| 29:RF:129:PHE:O   | 29:RF:142:TRP:CD1  | 2.62                     | 0.53              |
| 35:RP:14:LYS:O    | 35:RP:15:ARG:C     | 2.51                     | 0.53              |
| 35:RP:101:VAL:C   | 35:RP:103:ALA:H    | 2.17                     | 0.53              |
| 40:RU:86:ALA:HB1  | 40:RU:88:ILE:HD11  | 1.90                     | 0.53              |
| 41:RV:48:GLY:O    | 41:RV:49:THR:O     | 2.26                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:RW:8:ARG:HH11  | 42:RW:8:ARG:HG3   | 1.73                     | 0.53              |
| 42:RW:14:PRO:O    | 42:RW:17:VAL:N    | 2.42                     | 0.53              |
| 50:R4:42:PHE:O    | 50:R4:43:TYR:C    | 2.51                     | 0.53              |
| 52:R6:9:LEU:HD13  | 52:R6:26:ASN:ND2  | 2.24                     | 0.53              |
| 54:R8:52:LYS:N    | 54:R8:53:PRO:HD2  | 2.22                     | 0.53              |
| 1:XA:1126:U:H1'   | 1:XA:1280:A:C5    | 2.44                     | 0.53              |
| 1:XA:1129:C:N4    | 1:XA:1141:C:H42   | 2.05                     | 0.53              |
| 9:XI:4:TYR:CE2    | 9:XI:88:TYR:HB2   | 2.44                     | 0.53              |
| 11:XK:125:PHE:HD1 | 11:XK:125:PHE:N   | 2.05                     | 0.53              |
| 13:XM:76:ALA:O    | 13:XM:79:LYS:HB3  | 2.09                     | 0.53              |
| 15:XO:29:VAL:HG11 | 15:XO:67:LEU:HD21 | 1.89                     | 0.53              |
| 18:XR:36:ASN:O    | 18:XR:36:ASN:ND2  | 2.32                     | 0.53              |
| 29:YF:29:ASN:CB   | 29:YF:112:MET:HE1 | 2.38                     | 0.53              |
| 31:YH:12:PRO:HG3  | 31:YH:48:GLY:O    | 2.09                     | 0.53              |
| 33:YN:134:ARG:N   | 33:YN:135:PRO:CD  | 2.58                     | 0.53              |
| 35:YP:125:VAL:O   | 35:YP:145:PRO:HD2 | 2.08                     | 0.53              |
| 39:YT:34:VAL:CG1  | 39:YT:36:GLU:HG2  | 2.39                     | 0.53              |
| 43:YX:60:ARG:NH1  | 53:Y7:47:ARG:HH22 | 2.07                     | 0.53              |
| 47:Y1:20:ARG:HG2  | 47:Y1:20:ARG:NH1  | 2.24                     | 0.53              |
| 51:Y5:60:VAL:OXT  | 51:Y5:60:VAL:CG1  | 2.56                     | 0.53              |
| 52:Y6:9:LEU:HD13  | 52:Y6:26:ASN:ND2  | 2.24                     | 0.53              |
| 1:QA:243:A:H4'    | 1:QA:244:U:H3'    | 1.89                     | 0.53              |
| 1:QA:752:G:H1'    | 1:QA:754:C:H41    | 1.73                     | 0.53              |
| 1:QA:939:G:H5''   | 7:QG:102:ARG:NH1  | 2.24                     | 0.53              |
| 1:QA:1374:A:O2'   | 7:QG:28:ASN:HB3   | 2.08                     | 0.53              |
| 2:QB:5:ILE:N      | 2:QB:5:ILE:HD13   | 2.24                     | 0.53              |
| 2:QB:206:ASP:O    | 2:QB:207:ALA:HB3  | 2.08                     | 0.53              |
| 2:QB:233:SER:OG   | 2:QB:234:PRO:HD2  | 2.09                     | 0.53              |
| 4:QD:108:LEU:HD11 | 4:QD:174:LEU:CD2  | 2.37                     | 0.53              |
| 4:QD:172:PRO:HB2  | 4:QD:193:ASP:OD2  | 2.08                     | 0.53              |
| 4:QD:183:GLY:C    | 4:QD:184:LYS:HG3  | 2.34                     | 0.53              |
| 5:QE:36:ASP:OD1   | 5:QE:37:ARG:N     | 2.42                     | 0.53              |
| 7:QG:8:GLU:CD     | 7:QG:8:GLU:N      | 2.67                     | 0.53              |
| 13:QM:92:HIS:CD2  | 13:QM:98:VAL:HG21 | 2.43                     | 0.53              |
| 20:QT:30:LYS:HE2  | 20:QT:72:LEU:HD12 | 1.91                     | 0.53              |
| 21:QU:14:TRP:CZ3  | 21:QU:15:ARG:HD3  | 2.43                     | 0.53              |
| 22:QV:76:A:H2'    | 25:RA:2602:A:N6   | 2.24                     | 0.53              |
| 25:RA:2543:G:H21  | 25:RA:2646:C:H5'' | 1.73                     | 0.53              |
| 27:RD:43:ARG:NH1  | 27:RD:44:ASN:OD1  | 2.42                     | 0.53              |
| 28:RE:20:ALA:O    | 28:RE:21:VAL:CG2  | 2.48                     | 0.53              |
| 28:RE:25:VAL:HG11 | 39:RT:11:GLU:HG2  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:40:GLU:O     | 31:RH:41:MET:HB2   | 2.08                     | 0.53              |
| 31:RH:126:PRO:HD2  | 31:RH:127:GLU:H    | 1.72                     | 0.53              |
| 35:RP:12:ALA:C     | 35:RP:14:LYS:H     | 2.17                     | 0.53              |
| 38:RS:56:LEU:O     | 38:RS:58:LEU:HD22  | 2.09                     | 0.53              |
| 41:RV:51:VAL:CG1   | 41:RV:52:VAL:H     | 2.22                     | 0.53              |
| 47:R1:60:PHE:HE2   | 47:R1:91:LYS:HZ1   | 1.55                     | 0.53              |
| 52:R6:25:LYS:HE2   | 52:R6:27:LYS:HE3   | 1.91                     | 0.53              |
| 1:XA:738:C:H5''    | 6:XF:69:GLU:HB2    | 1.91                     | 0.53              |
| 4:XD:23:GLY:HA3    | 4:XD:112:VAL:CG2   | 2.38                     | 0.53              |
| 10:XJ:74:ILE:HD13  | 10:XJ:74:ILE:N     | 2.16                     | 0.53              |
| 12:XL:32:PHE:HE1   | 12:XL:86:ARG:HG3   | 1.73                     | 0.53              |
| 15:XO:7:GLU:O      | 15:XO:11:VAL:HG23  | 2.08                     | 0.53              |
| 25:YA:2846:G:OP2   | 39:YT:54:ARG:HB2   | 2.09                     | 0.53              |
| 27:YD:25:THR:O     | 27:YD:26:LYS:C     | 2.52                     | 0.53              |
| 27:YD:233:HIS:N    | 27:YD:233:HIS:CD2  | 2.75                     | 0.53              |
| 28:YE:119:ARG:HD3  | 28:YE:160:TYR:HB2  | 1.91                     | 0.53              |
| 31:YH:10:PRO:C     | 31:YH:11:VAL:HG22  | 2.34                     | 0.53              |
| 31:YH:139:GLN:O    | 31:YH:143:GLN:HB2  | 2.09                     | 0.53              |
| 33:YN:95:PRO:O     | 33:YN:96:GLU:C     | 2.51                     | 0.53              |
| 35:YP:101:VAL:C    | 35:YP:103:ALA:H    | 2.17                     | 0.53              |
| 35:YP:125:VAL:O    | 35:YP:125:VAL:HG13 | 2.09                     | 0.53              |
| 36:YQ:81:VAL:C     | 36:YQ:82:ARG:CG    | 2.76                     | 0.53              |
| 38:YS:56:LEU:O     | 38:YS:58:LEU:HD22  | 2.09                     | 0.53              |
| 39:YT:3:ARG:HG3    | 39:YT:7:ILE:CG1    | 2.36                     | 0.53              |
| 45:YZ:141:VAL:HG23 | 45:YZ:144:LEU:HB2  | 1.90                     | 0.53              |
| 50:Y4:36:CYS:O     | 50:Y4:37:SER:C     | 2.52                     | 0.53              |
| 52:Y6:7:ILE:CG1    | 52:Y6:8:LYS:H      | 2.07                     | 0.53              |
| 2:QB:140:HIS:C     | 2:QB:142:LEU:H     | 2.16                     | 0.53              |
| 2:QB:200:ILE:HG22  | 2:QB:201:ILE:N     | 2.24                     | 0.53              |
| 7:QG:95:ARG:CZ     | 7:QG:99:LEU:HD11   | 2.38                     | 0.53              |
| 9:QI:53:VAL:CB     | 9:QI:95:LYS:HE3    | 2.36                     | 0.53              |
| 16:QP:72:ARG:HD3   | 16:QP:73:LEU:HD23  | 1.91                     | 0.53              |
| 17:QQ:65:ILE:HD12  | 17:QQ:65:ILE:H     | 1.74                     | 0.53              |
| 18:QR:44:LEU:HD12  | 18:QR:44:LEU:N     | 2.24                     | 0.53              |
| 23:QY:41:A:O2'     | 23:QY:42:G:OP1     | 2.21                     | 0.53              |
| 25:RA:620:G:H4'    | 25:RA:621:A:H5''   | 1.91                     | 0.53              |
| 26:RB:40:U:H1'     | 26:RB:45:A:H61     | 1.73                     | 0.53              |
| 27:RD:25:THR:O     | 27:RD:26:LYS:C     | 2.52                     | 0.53              |
| 27:RD:25:THR:HG21  | 27:RD:82:ILE:H     | 1.70                     | 0.53              |
| 27:RD:34:VAL:O     | 27:RD:34:VAL:CG1   | 2.50                     | 0.53              |
| 27:RD:155:LEU:CD1  | 27:RD:155:LEU:N    | 2.71                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:10:PRO:C     | 31:RH:11:VAL:HG22  | 2.34                     | 0.53              |
| 33:RN:18:ALA:O     | 33:RN:19:GLU:C     | 2.52                     | 0.53              |
| 33:RN:75:TYR:C     | 33:RN:76:SER:O     | 2.52                     | 0.53              |
| 35:RP:79:ARG:HD3   | 35:RP:110:TYR:CE1  | 2.43                     | 0.53              |
| 35:RP:125:VAL:O    | 35:RP:125:VAL:HG13 | 2.09                     | 0.53              |
| 36:RQ:7:MET:HE1    | 36:RQ:73:PRO:HG3   | 1.91                     | 0.53              |
| 37:RR:33:ARG:NH2   | 51:R5:55:ARG:CG    | 2.66                     | 0.53              |
| 37:RR:107:ASP:C    | 37:RR:107:ASP:OD2  | 2.52                     | 0.53              |
| 48:R2:41:ILE:HD11  | 48:R2:44:LEU:HB2   | 1.90                     | 0.53              |
| 1:XA:939:G:H5''    | 7:XG:102:ARG:HH12  | 1.74                     | 0.53              |
| 1:XA:1179:A:O3'    | 9:XI:103:THR:HG23  | 2.08                     | 0.53              |
| 3:XC:51:GLY:O      | 3:XC:70:VAL:HG13   | 2.09                     | 0.53              |
| 3:XC:134:ILE:CG2   | 3:XC:168:ALA:HB3   | 2.39                     | 0.53              |
| 6:XF:75:LEU:HD21   | 6:XF:79:LEU:HD11   | 1.91                     | 0.53              |
| 8:XH:87:SER:HA     | 8:XH:93:VAL:HG23   | 1.91                     | 0.53              |
| 9:XI:113:LYS:HD3   | 9:XI:119:ALA:O     | 2.09                     | 0.53              |
| 13:XM:8:GLU:C      | 13:XM:9:ILE:HG23   | 2.34                     | 0.53              |
| 15:XO:26:GLU:HA    | 15:XO:81:LEU:HD22  | 1.90                     | 0.53              |
| 15:XO:62:GLN:N     | 15:XO:65:ARG:HH12  | 2.06                     | 0.53              |
| 25:YA:270(T):G:OP1 | 47:Y1:97:LEU:HD13  | 2.09                     | 0.53              |
| 25:YA:576:U:H2'    | 25:YA:577:G:C8     | 2.44                     | 0.53              |
| 25:YA:1916:A:H2'   | 25:YA:1917:U:O4'   | 2.09                     | 0.53              |
| 25:YA:2845:G:H5''  | 39:YT:55:ASN:HA    | 1.91                     | 0.53              |
| 28:YE:7:VAL:O      | 28:YE:196:VAL:HG13 | 2.09                     | 0.53              |
| 28:YE:64:LYS:C     | 28:YE:66:HIS:N     | 2.67                     | 0.53              |
| 29:YF:9:ILE:HD11   | 29:YF:125:LEU:CG   | 2.36                     | 0.53              |
| 29:YF:129:PHE:O    | 29:YF:142:TRP:CD1  | 2.62                     | 0.53              |
| 30:YG:97:ASP:H     | 30:YG:100:TRP:CD1  | 2.19                     | 0.53              |
| 31:YH:44:VAL:O     | 31:YH:44:VAL:CG2   | 2.57                     | 0.53              |
| 32:YI:79:ILE:N     | 32:YI:141:LYS:O    | 2.42                     | 0.53              |
| 33:YN:131:GLN:CG   | 33:YN:132:ALA:H    | 2.20                     | 0.53              |
| 37:YR:1:MET:O      | 37:YR:2:ARG:HG3    | 2.08                     | 0.53              |
| 38:YS:56:LEU:C     | 38:YS:56:LEU:HD23  | 2.34                     | 0.53              |
| 40:YU:92:ARG:NH2   | 40:YU:94:ASN:HD22  | 2.07                     | 0.53              |
| 41:YV:7:THR:CG2    | 41:YV:22:VAL:HG11  | 2.39                     | 0.53              |
| 41:YV:38:LEU:HD13  | 41:YV:55:ALA:HB3   | 1.91                     | 0.53              |
| 43:YX:53:LYS:NZ    | 43:YX:55:ASN:HD21  | 2.06                     | 0.53              |
| 50:Y4:56:VAL:HA    | 50:Y4:60:GLN:CB    | 2.29                     | 0.53              |
| 52:Y6:25:LYS:HE2   | 52:Y6:27:LYS:HE3   | 1.91                     | 0.53              |
| 1:QA:355:C:H1'     | 1:QA:388:G:H2'     | 1.90                     | 0.52              |
| 1:QA:1356:G:H2'    | 1:QA:1357:A:C8     | 2.44                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:QD:163:GLU:C    | 4:QD:165:MET:N     | 2.66                     | 0.52              |
| 4:QD:206:PHE:HD2  | 4:QD:207:TYR:CD1   | 2.27                     | 0.52              |
| 5:QE:10:MET:HE2   | 5:QE:13:ILE:HD13   | 1.90                     | 0.52              |
| 6:QF:89:MET:O     | 6:QF:90:VAL:C      | 2.51                     | 0.52              |
| 8:QH:33:GLU:C     | 8:QH:35:ILE:N      | 2.65                     | 0.52              |
| 13:QM:73:GLU:O    | 13:QM:76:ALA:N     | 2.42                     | 0.52              |
| 13:QM:117:VAL:O   | 13:QM:118:ALA:C    | 2.51                     | 0.52              |
| 15:QO:39:LEU:O    | 15:QO:40:SER:C     | 2.50                     | 0.52              |
| 18:QR:29:PHE:CD2  | 18:QR:29:PHE:N     | 2.76                     | 0.52              |
| 22:QV:4:G:HO2'    | 22:QV:5:G:H8       | 1.56                     | 0.52              |
| 22:QV:15:G:H22    | 22:QV:48:C:H42     | 1.57                     | 0.52              |
| 25:RA:2713:A:OP1  | 37:RR:14:SER:OG    | 2.27                     | 0.52              |
| 27:RD:130:ALA:C   | 27:RD:131:LEU:HD12 | 2.33                     | 0.52              |
| 36:RQ:76:LYS:O    | 36:RQ:88:GLY:HA3   | 2.09                     | 0.52              |
| 39:RT:55:ASN:O    | 39:RT:57:PHE:O     | 2.26                     | 0.52              |
| 49:R3:9:VAL:HG12  | 49:R3:32:GLN:HE22  | 1.74                     | 0.52              |
| 50:R4:47:GLN:O    | 50:R4:48:ARG:HB2   | 2.07                     | 0.52              |
| 50:R4:54:GLY:O    | 50:R4:71:ARG:HA    | 2.08                     | 0.52              |
| 52:R6:13:CYS:O    | 52:R6:14:THR:HB    | 2.08                     | 0.52              |
| 54:R8:43:GLN:C    | 54:R8:44:LYS:HD2   | 2.34                     | 0.52              |
| 1:XA:715:A:H2'    | 1:XA:716:A:C8      | 2.45                     | 0.52              |
| 1:XA:1158:C:H4'   | 2:XB:133:LYS:NZ    | 2.24                     | 0.52              |
| 2:XB:9:GLU:OE2    | 2:XB:9:GLU:N       | 2.42                     | 0.52              |
| 2:XB:188:ALA:HB3  | 2:XB:200:ILE:CG2   | 2.40                     | 0.52              |
| 5:XE:12:LEU:O     | 5:XE:13:ILE:HD12   | 2.08                     | 0.52              |
| 5:XE:140:ARG:HB2  | 5:XE:140:ARG:NH1   | 2.23                     | 0.52              |
| 8:XH:100:ILE:CB   | 8:XH:125:ARG:HH12  | 2.20                     | 0.52              |
| 11:XK:115:PRO:C   | 11:XK:117:ASN:H    | 2.17                     | 0.52              |
| 13:XM:87:TYR:CE1  | 13:XM:91:ARG:HD3   | 2.44                     | 0.52              |
| 19:XS:11:VAL:O    | 19:XS:11:VAL:HG13  | 2.09                     | 0.52              |
| 25:YA:2250:G:C5   | 36:YQ:82:ARG:HD2   | 2.44                     | 0.52              |
| 25:YA:2712:U:H1'  | 25:YA:2712(A):A:C8 | 2.44                     | 0.52              |
| 28:YE:39:PRO:HG2  | 28:YE:40:GLU:OE1   | 2.09                     | 0.52              |
| 29:YF:34:TRP:CH2  | 35:YP:8:PRO:HB3    | 2.43                     | 0.52              |
| 30:YG:111:LEU:HB2 | 50:Y4:38:LYS:HZ3   | 1.72                     | 0.52              |
| 35:YP:147:LEU:O   | 35:YP:148:LEU:CB   | 2.57                     | 0.52              |
| 37:YR:70:LEU:O    | 37:YR:72:ASP:N     | 2.43                     | 0.52              |
| 37:YR:107:ASP:C   | 37:YR:107:ASP:OD2  | 2.52                     | 0.52              |
| 44:YY:88:LYS:HZ2  | 44:YY:88:LYS:HA    | 1.71                     | 0.52              |
| 47:Y1:25:LYS:C    | 47:Y1:27:GLU:H     | 2.17                     | 0.52              |
| 1:QA:34:C:H2'     | 1:QA:35:G:H8       | 1.74                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:939:G:H5''    | 7:QG:102:ARG:HH12 | 1.74                     | 0.52              |
| 1:QA:1244:C:H42    | 1:QA:1293:G:H1    | 1.55                     | 0.52              |
| 1:QA:1318:A:H4'    | 19:QS:11:VAL:CG1  | 2.38                     | 0.52              |
| 1:QA:1348:U:N3     | 1:QA:1374:A:H2    | 2.07                     | 0.52              |
| 2:QB:102:LEU:HB3   | 2:QB:180:LEU:HD12 | 1.90                     | 0.52              |
| 3:QC:134:ILE:CG2   | 3:QC:168:ALA:HB3  | 2.39                     | 0.52              |
| 4:QD:27:TYR:OH     | 6:XF:15:ASP:OD2   | 2.18                     | 0.52              |
| 4:QD:120:LEU:HD22  | 4:QD:125:HIS:CB   | 2.38                     | 0.52              |
| 8:QH:87:SER:HA     | 8:QH:93:VAL:HG23  | 1.91                     | 0.52              |
| 12:QL:27:LEU:C     | 12:QL:29:GLY:N    | 2.64                     | 0.52              |
| 13:QM:82:MET:HE3   | 13:QM:93:ARG:HG2  | 1.91                     | 0.52              |
| 16:QP:1:MET:SD     | 16:QP:3:LYS:HE3   | 2.49                     | 0.52              |
| 25:RA:221:A:H4'    | 25:RA:222:A:O5'   | 2.09                     | 0.52              |
| 25:RA:1161:C:O2'   | 41:RV:8:GLY:HA2   | 2.09                     | 0.52              |
| 25:RA:2022:U:O2'   | 25:RA:2617:C:H5'  | 2.10                     | 0.52              |
| 25:RA:2361:A:O5'   | 54:R8:27:THR:OG1  | 2.25                     | 0.52              |
| 25:RA:2404:C:H1'   | 35:RP:67:MET:CE   | 2.38                     | 0.52              |
| 29:RF:125:LEU:HA   | 29:RF:194:MET:O   | 2.10                     | 0.52              |
| 31:RH:44:VAL:O     | 31:RH:44:VAL:CG2  | 2.57                     | 0.52              |
| 32:RI:76:THR:OG1   | 32:RI:139:GLN:OE1 | 2.18                     | 0.52              |
| 33:RN:12:ARG:NH1   | 33:RN:50:ASP:OD2  | 2.41                     | 0.52              |
| 33:RN:94:HIS:O     | 33:RN:95:PRO:O    | 2.27                     | 0.52              |
| 38:RS:56:LEU:C     | 38:RS:56:LEU:HD23 | 2.34                     | 0.52              |
| 38:RS:89:ARG:HH11  | 38:RS:89:ARG:HG2  | 1.74                     | 0.52              |
| 39:RT:14:TYR:CD1   | 39:RT:14:TYR:N    | 2.77                     | 0.52              |
| 39:RT:100:TYR:HB3  | 39:RT:103:ARG:NH1 | 2.25                     | 0.52              |
| 1:XA:312:C:H2'     | 1:XA:313:A:C8     | 2.45                     | 0.52              |
| 3:XC:48:TYR:O      | 3:XC:51:GLY:N     | 2.41                     | 0.52              |
| 6:XF:86:ARG:O      | 6:XF:87:ARG:CG    | 2.50                     | 0.52              |
| 14:XN:7:ILE:CG1    | 14:XN:8:GLU:N     | 2.72                     | 0.52              |
| 19:XS:27:GLU:O     | 19:XS:28:LYS:CG   | 2.53                     | 0.52              |
| 19:XS:29:ARG:HD3   | 19:XS:30:LEU:HD13 | 1.91                     | 0.52              |
| 25:YA:993:G:OP1    | 40:YU:50:ARG:NH1  | 2.43                     | 0.52              |
| 25:YA:2308:G:N2    | 25:YA:2311:A:H2   | 2.01                     | 0.52              |
| 27:YD:35:LYS:HD3   | 27:YD:63:ARG:CA   | 2.39                     | 0.52              |
| 27:YD:155:LEU:CD1  | 27:YD:155:LEU:N   | 2.71                     | 0.52              |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:CE  | 2.34                     | 0.52              |
| 30:YG:16:ARG:HH11  | 30:YG:16:ARG:HG2  | 1.74                     | 0.52              |
| 30:YG:179:PRO:HG3  | 50:Y4:38:LYS:HZ1  | 1.74                     | 0.52              |
| 33:YN:18:ALA:O     | 33:YN:19:GLU:C    | 2.52                     | 0.52              |
| 33:YN:109:LYS:HD2  | 33:YN:109:LYS:H   | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:94:ALA:O     | 39:YT:95:ARG:HB3   | 2.09                     | 0.52              |
| 42:YW:7:ALA:HB2    | 42:YW:50:VAL:CG2   | 2.40                     | 0.52              |
| 42:YW:25:ARG:HB2   | 42:YW:25:ARG:HH11  | 1.74                     | 0.52              |
| 49:Y3:6:VAL:HG12   | 49:Y3:56:VAL:HG22  | 1.92                     | 0.52              |
| 50:Y4:15:ILE:HD13  | 50:Y4:15:ILE:H     | 1.73                     | 0.52              |
| 50:Y4:23:GLU:C     | 50:Y4:24:THR:HG1   | 2.17                     | 0.52              |
| 1:QA:186:C:H2'     | 1:QA:186(A):C:C6   | 2.45                     | 0.52              |
| 1:QA:323:U:H5'     | 20:QT:23:ARG:HB2   | 1.91                     | 0.52              |
| 1:QA:542:G:OP1     | 4:QD:10:ARG:NH2    | 2.41                     | 0.52              |
| 1:QA:1231:G:O3'    | 9:QI:126:SER:OG    | 2.27                     | 0.52              |
| 3:QC:29:TYR:OH     | 14:QN:54:PRO:HD2   | 2.09                     | 0.52              |
| 13:QM:8:GLU:C      | 13:QM:9:ILE:HG23   | 2.34                     | 0.52              |
| 13:QM:87:TYR:CE1   | 13:QM:91:ARG:HD3   | 2.44                     | 0.52              |
| 15:QO:26:GLU:HA    | 15:QO:81:LEU:HD22  | 1.90                     | 0.52              |
| 19:QS:11:VAL:O     | 19:QS:11:VAL:HG13  | 2.10                     | 0.52              |
| 25:RA:520:G:H2'    | 25:RA:521:G:C8     | 2.45                     | 0.52              |
| 25:RA:586:A:H5'    | 29:RF:89:VAL:HG21  | 1.91                     | 0.52              |
| 25:RA:859:G:O2'    | 25:RA:860:U:O2     | 2.21                     | 0.52              |
| 25:RA:1009:A:OP1   | 33:RN:37:LYS:NZ    | 2.42                     | 0.52              |
| 25:RA:1169:G:H1    | 25:RA:1180:C:H42   | 1.56                     | 0.52              |
| 25:RA:2215:G:H2'   | 25:RA:2216:G:H8    | 1.74                     | 0.52              |
| 25:RA:2725:A:O2'   | 25:RA:2726:U:H5''  | 2.08                     | 0.52              |
| 28:RE:7:VAL:O      | 28:RE:196:VAL:HG13 | 2.09                     | 0.52              |
| 28:RE:61:ARG:O     | 28:RE:63:LEU:N     | 2.42                     | 0.52              |
| 28:RE:64:LYS:C     | 28:RE:66:HIS:N     | 2.68                     | 0.52              |
| 29:RF:140:LEU:O    | 29:RF:143:ALA:HB3  | 2.09                     | 0.52              |
| 31:RH:12:PRO:HG3   | 31:RH:48:GLY:O     | 2.09                     | 0.52              |
| 35:RP:92:GLU:HA    | 35:RP:123:LEU:CD2  | 2.39                     | 0.52              |
| 36:RQ:29:PHE:HB3   | 36:RQ:65:PHE:CZ    | 2.44                     | 0.52              |
| 39:RT:110:ILE:HG23 | 39:RT:111:ARG:N    | 2.24                     | 0.52              |
| 42:RW:32:ALA:O     | 42:RW:33:ARG:C     | 2.52                     | 0.52              |
| 47:R1:29:GLY:C     | 47:R1:30:VAL:CG2   | 2.82                     | 0.52              |
| 47:R1:85:LEU:HA    | 47:R1:87:PRO:HD2   | 1.92                     | 0.52              |
| 50:R4:49:PHE:N     | 50:R4:49:PHE:CD1   | 2.76                     | 0.52              |
| 51:R5:55:ARG:HG3   | 51:R5:57:VAL:H     | 1.74                     | 0.52              |
| 1:XA:129(A):G:O2'  | 1:XA:189:U:H3'     | 2.08                     | 0.52              |
| 1:XA:703:G:O2'     | 1:XA:704:A:OP2     | 2.26                     | 0.52              |
| 1:XA:791:G:H2'     | 1:XA:792:A:H5'     | 1.91                     | 0.52              |
| 3:XC:173:VAL:HG12  | 3:XC:173:VAL:O     | 2.08                     | 0.52              |
| 4:XD:163:GLU:C     | 4:XD:165:MET:N     | 2.66                     | 0.52              |
| 4:XD:206:PHE:HD2   | 4:XD:207:TYR:CD1   | 2.27                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:XE:36:ASP:OD1    | 5:XE:37:ARG:N     | 2.42                     | 0.52              |
| 7:XG:106:GLN:O     | 7:XG:110:GLN:HG3  | 2.10                     | 0.52              |
| 10:XJ:39:PRO:HB3   | 10:XJ:70:ARG:NH1  | 2.24                     | 0.52              |
| 17:XQ:62:SER:HB3   | 17:XQ:72:ARG:HH21 | 1.72                     | 0.52              |
| 25:YA:1007:C:OP1   | 33:YN:35:ARG:NH1  | 2.40                     | 0.52              |
| 25:YA:2724:C:P     | 37:YR:1:MET:HE3   | 2.49                     | 0.52              |
| 28:YE:7:VAL:CG2    | 28:YE:8:LYS:H     | 2.11                     | 0.52              |
| 29:YF:140:LEU:O    | 29:YF:143:ALA:HB3 | 2.09                     | 0.52              |
| 31:YH:89:ILE:O     | 31:YH:89:ILE:CG1  | 2.57                     | 0.52              |
| 33:YN:75:TYR:C     | 33:YN:76:SER:O    | 2.52                     | 0.52              |
| 34:YO:107:ARG:CA   | 34:YO:112:MET:HE1 | 2.39                     | 0.52              |
| 35:YP:37:GLY:HA2   | 35:YP:41:ARG:NE   | 2.24                     | 0.52              |
| 36:YQ:29:PHE:HB3   | 36:YQ:65:PHE:CZ   | 2.44                     | 0.52              |
| 41:YV:35:LEU:HD21  | 41:YV:57:VAL:CG2  | 2.30                     | 0.52              |
| 42:YW:8:ARG:HG3    | 42:YW:8:ARG:HH11  | 1.73                     | 0.52              |
| 42:YW:38:TYR:OH    | 51:Y5:47:PRO:HG3  | 2.08                     | 0.52              |
| 47:Y1:4:VAL:HG22   | 47:Y1:5:CYS:N     | 2.24                     | 0.52              |
| 48:Y2:50:ILE:CD1   | 48:Y2:51:ARG:N    | 2.61                     | 0.52              |
| 50:Y4:40:HIS:N     | 50:Y4:41:PRO:CD   | 2.73                     | 0.52              |
| 1:QA:302:G:O3'     | 12:QL:17:LYS:HE2  | 2.10                     | 0.52              |
| 1:QA:1080:A:H5''   | 5:QE:16:THR:HG21  | 1.91                     | 0.52              |
| 1:QA:1314:C:H5     | 19:QS:4:SER:HB2   | 1.75                     | 0.52              |
| 2:QB:9:GLU:N       | 2:QB:9:GLU:OE2    | 2.42                     | 0.52              |
| 4:QD:176:LEU:HD12  | 4:QD:182:LYS:O    | 2.10                     | 0.52              |
| 6:QF:89:MET:O      | 6:QF:89:MET:HG2   | 2.09                     | 0.52              |
| 7:QG:44:TYR:C      | 7:QG:46:ALA:N     | 2.66                     | 0.52              |
| 8:QH:100:ILE:CB    | 8:QH:125:ARG:HH12 | 2.20                     | 0.52              |
| 15:QO:62:GLN:N     | 15:QO:65:ARG:HH12 | 2.06                     | 0.52              |
| 19:QS:65:ASN:ND2   | 19:QS:65:ASN:H    | 2.08                     | 0.52              |
| 25:RA:137(A):G:H1' | 43:RX:41:ASN:HD22 | 1.75                     | 0.52              |
| 25:RA:309:G:N3     | 25:RA:329:G:O2'   | 2.41                     | 0.52              |
| 25:RA:519:U:H2'    | 25:RA:520:G:C8    | 2.45                     | 0.52              |
| 27:RD:77:ALA:HB2   | 27:RD:97:TYR:CG   | 2.44                     | 0.52              |
| 29:RF:53:THR:C     | 29:RF:55:GLY:N    | 2.67                     | 0.52              |
| 33:RN:7:LYS:HD3    | 33:RN:9:VAL:CA    | 2.38                     | 0.52              |
| 38:RS:86:ALA:O     | 38:RS:87:PHE:HB3  | 2.10                     | 0.52              |
| 38:RS:106:ARG:HA   | 38:RS:110:LEU:CG  | 2.39                     | 0.52              |
| 40:RU:88:ILE:H     | 40:RU:88:ILE:CD1  | 2.05                     | 0.52              |
| 40:RU:91:ASP:O     | 40:RU:92:ARG:C    | 2.53                     | 0.52              |
| 41:RV:48:GLY:O     | 41:RV:49:THR:C    | 2.52                     | 0.52              |
| 49:R3:21:ALA:O     | 49:R3:25:ALA:N    | 2.41                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 49:R3:56:VAL:CG1   | 49:R3:57:GLU:H    | 2.19                     | 0.52              |
| 1:XA:1194:U:H4'    | 5:XE:22:GLY:O     | 2.10                     | 0.52              |
| 1:XA:1297:C:O2'    | 1:XA:1298:C:O5'   | 2.27                     | 0.52              |
| 2:XB:80:ILE:CD1    | 2:XB:208:ILE:HG23 | 2.22                     | 0.52              |
| 2:XB:92:TYR:CE1    | 2:XB:151:GLY:HA3  | 2.45                     | 0.52              |
| 2:XB:232:PRO:O     | 2:XB:233:SER:O    | 2.27                     | 0.52              |
| 2:XB:233:SER:OG    | 2:XB:234:PRO:HD2  | 2.09                     | 0.52              |
| 9:XI:128:ARG:NH2   | 22:XV:35:A:OP2    | 2.43                     | 0.52              |
| 10:XJ:4:ILE:HB     | 10:XJ:74:ILE:CD1  | 2.36                     | 0.52              |
| 11:XK:62:GLN:O     | 11:XK:63:LEU:C    | 2.51                     | 0.52              |
| 13:XM:82:MET:HE3   | 13:XM:93:ARG:HG2  | 1.91                     | 0.52              |
| 25:YA:528:A:O2'    | 25:YA:529:A:H5'   | 2.09                     | 0.52              |
| 25:YA:1359:A:H61   | 25:YA:1372:U:H3   | 1.57                     | 0.52              |
| 25:YA:1957:C:H2'   | 25:YA:1958:C:C6   | 2.45                     | 0.52              |
| 25:YA:2334:G:C6    | 46:Y0:75:LEU:HD21 | 2.44                     | 0.52              |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:NH2 | 2.25                     | 0.52              |
| 29:YF:196:LEU:C    | 29:YF:197:ASP:O   | 2.50                     | 0.52              |
| 31:YH:24:VAL:HG23  | 31:YH:24:VAL:O    | 2.09                     | 0.52              |
| 31:YH:121:ILE:HG12 | 31:YH:135:GLY:HA3 | 1.91                     | 0.52              |
| 33:YN:57:ALA:O     | 33:YN:58:ASP:HB3  | 2.09                     | 0.52              |
| 38:YS:62:LYS:HB3   | 38:YS:97:ARG:CD   | 2.39                     | 0.52              |
| 39:YT:100:TYR:HB3  | 39:YT:103:ARG:NH1 | 2.25                     | 0.52              |
| 41:YV:34:GLU:O     | 41:YV:36:PRO:HD3  | 2.09                     | 0.52              |
| 42:YW:32:ALA:O     | 42:YW:33:ARG:C    | 2.52                     | 0.52              |
| 44:YY:61:ILE:HG23  | 44:YY:62:GLU:N    | 2.24                     | 0.52              |
| 44:YY:91:GLU:HG3   | 44:YY:92:ASN:N    | 2.25                     | 0.52              |
| 49:Y3:9:VAL:HG12   | 49:Y3:32:GLN:HE22 | 1.74                     | 0.52              |
| 52:Y6:14:THR:OG1   | 52:Y6:19:ARG:NE   | 2.41                     | 0.52              |
| 1:QA:327:A:O2'     | 1:QA:328:C:O4'    | 2.23                     | 0.52              |
| 1:QA:719:C:C2      | 18:QR:50:ILE:HD13 | 2.45                     | 0.52              |
| 2:QB:188:ALA:HB3   | 2:QB:200:ILE:CG2  | 2.40                     | 0.52              |
| 4:QD:10:ARG:O      | 4:QD:14:ARG:HB2   | 2.08                     | 0.52              |
| 4:QD:106:TYR:CE1   | 4:QD:112:VAL:O    | 2.62                     | 0.52              |
| 5:QE:87:SER:HB3    | 5:QE:131:ILE:CD1  | 2.38                     | 0.52              |
| 9:QI:113:LYS:HD3   | 9:QI:119:ALA:O    | 2.09                     | 0.52              |
| 10:QJ:4:ILE:HB     | 10:QJ:74:ILE:CD1  | 2.37                     | 0.52              |
| 11:QK:91:ARG:NH2   | 18:QR:88:LYS:NZ   | 2.58                     | 0.52              |
| 12:QL:127:GLU:O    | 12:QL:128:ALA:HB3 | 2.10                     | 0.52              |
| 20:QT:13:LEU:HD12  | 20:QT:13:LEU:C    | 2.34                     | 0.52              |
| 25:RA:2308:G:H22   | 25:RA:2311:A:H2   | 1.56                     | 0.52              |
| 25:RA:2415:G:H4'   | 35:RP:67:MET:N    | 2.25                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:RD:134:ARG:HB2 | 27:RD:135:PHE:HD2 | 1.75                     | 0.52              |
| 27:RD:210:GLY:O   | 27:RD:213:ARG:N   | 2.43                     | 0.52              |
| 30:RG:16:ARG:HH11 | 30:RG:16:ARG:HG2  | 1.74                     | 0.52              |
| 33:RN:56:ASN:ND2  | 33:RN:125:GLY:C   | 2.66                     | 0.52              |
| 33:RN:68:GLU:HG2  | 33:RN:88:GLU:CD   | 2.33                     | 0.52              |
| 33:RN:103:VAL:O   | 33:RN:106:MET:N   | 2.42                     | 0.52              |
| 35:RP:64:LYS:C    | 35:RP:66:GLY:N    | 2.56                     | 0.52              |
| 47:R1:20:ARG:HG2  | 47:R1:20:ARG:NH1  | 2.24                     | 0.52              |
| 50:R4:36:CYS:O    | 50:R4:37:SER:C    | 2.52                     | 0.52              |
| 50:R4:48:ARG:CZ   | 50:R4:51:ASP:HA   | 2.40                     | 0.52              |
| 1:XA:38:G:H22     | 1:XA:397:A:H5''   | 1.73                     | 0.52              |
| 1:XA:503:C:OP2    | 12:XL:116:SER:HB3 | 2.09                     | 0.52              |
| 2:XB:87:ARG:HH11  | 2:XB:223:ILE:HD12 | 1.73                     | 0.52              |
| 2:XB:170:GLU:C    | 2:XB:172:ILE:HD12 | 2.33                     | 0.52              |
| 7:XG:8:GLU:CD     | 7:XG:8:GLU:N      | 2.67                     | 0.52              |
| 11:XK:91:ARG:NH2  | 18:XR:88:LYS:NZ   | 2.57                     | 0.52              |
| 19:XS:65:ASN:ND2  | 19:XS:65:ASN:H    | 2.08                     | 0.52              |
| 20:XT:13:LEU:HD12 | 20:XT:13:LEU:C    | 2.34                     | 0.52              |
| 25:YA:954:G:OP1   | 36:YQ:15:GLY:N    | 2.37                     | 0.52              |
| 25:YA:1032:A:O3'  | 55:Y9:16:VAL:HG11 | 2.10                     | 0.52              |
| 25:YA:2832:U:H4'  | 25:YA:2833:G:H5'' | 1.91                     | 0.52              |
| 27:YD:36:PRO:HA   | 27:YD:62:TYR:O    | 2.09                     | 0.52              |
| 27:YD:66:ASP:OD2  | 27:YD:69:ARG:HG2  | 2.09                     | 0.52              |
| 28:YE:93:VAL:C    | 28:YE:95:ILE:H    | 2.17                     | 0.52              |
| 28:YE:137:HIS:HB3 | 28:YE:138:PRO:CD  | 2.37                     | 0.52              |
| 29:YF:132:VAL:O   | 29:YF:133:ASN:C   | 2.52                     | 0.52              |
| 30:YG:124:SER:HB2 | 30:YG:131:TYR:CE1 | 2.44                     | 0.52              |
| 33:YN:103:VAL:O   | 33:YN:106:MET:N   | 2.42                     | 0.52              |
| 34:YO:79:PHE:CD2  | 39:YT:72:VAL:HG22 | 2.45                     | 0.52              |
| 37:YR:52:ILE:CG2  | 37:YR:94:TYR:HD1  | 2.22                     | 0.52              |
| 39:YT:36:GLU:O    | 39:YT:37:GLY:C    | 2.53                     | 0.52              |
| 48:Y2:7:ARG:HG3   | 48:Y2:7:ARG:NH1   | 2.25                     | 0.52              |
| 50:Y4:48:ARG:CZ   | 50:Y4:51:ASP:HA   | 2.40                     | 0.52              |
| 50:Y4:54:GLY:O    | 50:Y4:71:ARG:HA   | 2.08                     | 0.52              |
| 52:Y6:30:THR:O    | 52:Y6:30:THR:HG23 | 2.09                     | 0.52              |
| 54:Y8:61:LEU:O    | 54:Y8:62:LEU:CB   | 2.57                     | 0.52              |
| 1:QA:375:U:H4'    | 16:QP:17:TYR:CE2  | 2.39                     | 0.52              |
| 1:QA:1112:C:H1'   | 3:QC:179:ARG:NH1  | 2.25                     | 0.52              |
| 1:QA:1305:G:H22   | 1:QA:1331:G:H2'   | 1.75                     | 0.52              |
| 3:QC:140:ARG:HG3  | 3:QC:140:ARG:HH11 | 1.75                     | 0.52              |
| 4:QD:31:CYS:O     | 4:QD:32:ALA:HB3   | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:QF:22:GLU:CD     | 6:QF:82:ARG:HH21   | 2.18                     | 0.52              |
| 7:QG:151:TYR:HA    | 7:QG:153:HIS:CE1   | 2.45                     | 0.52              |
| 16:QP:34:GLU:OE1   | 16:QP:55:ARG:HD3   | 2.10                     | 0.52              |
| 19:QS:50:ALA:CB    | 19:QS:57:HIS:HB3   | 2.37                     | 0.52              |
| 25:RA:2051:A:OP1   | 28:RE:137:HIS:ND1  | 2.39                     | 0.52              |
| 27:RD:66:ASP:OD2   | 27:RD:69:ARG:HG2   | 2.09                     | 0.52              |
| 28:RE:39:PRO:HG2   | 28:RE:40:GLU:OE1   | 2.09                     | 0.52              |
| 30:RG:124:SER:HB2  | 30:RG:131:TYR:CE1  | 2.44                     | 0.52              |
| 31:RH:121:ILE:HG12 | 31:RH:135:GLY:HA3  | 1.91                     | 0.52              |
| 38:RS:83:LYS:O     | 38:RS:109:GLY:CA   | 2.46                     | 0.52              |
| 38:RS:95:HIS:CG    | 38:RS:96:GLY:N     | 2.77                     | 0.52              |
| 41:RV:34:GLU:O     | 41:RV:36:PRO:HD3   | 2.10                     | 0.52              |
| 41:RV:41:GLY:HA3   | 41:RV:46:VAL:CG1   | 2.38                     | 0.52              |
| 50:R4:55:ARG:C     | 50:R4:59:PHE:HB3   | 2.35                     | 0.52              |
| 2:XB:82:ARG:HB3    | 2:XB:83:MET:HE2    | 1.92                     | 0.52              |
| 4:XD:176:LEU:HD12  | 4:XD:182:LYS:O     | 2.10                     | 0.52              |
| 4:XD:183:GLY:C     | 4:XD:184:LYS:HG3   | 2.34                     | 0.52              |
| 6:XF:89:MET:O      | 6:XF:90:VAL:C      | 2.51                     | 0.52              |
| 7:XG:44:TYR:C      | 7:XG:46:ALA:N      | 2.66                     | 0.52              |
| 9:XI:13:ALA:HB2    | 9:XI:68:GLY:HA3    | 1.91                     | 0.52              |
| 10:XJ:6:ILE:CG2    | 10:XJ:98:ILE:HG13  | 2.21                     | 0.52              |
| 13:XM:73:GLU:O     | 13:XM:76:ALA:N     | 2.42                     | 0.52              |
| 15:XO:61:GLY:C     | 15:XO:65:ARG:NH1   | 2.67                     | 0.52              |
| 16:XP:4:ILE:HD12   | 16:XP:4:ILE:N      | 2.23                     | 0.52              |
| 16:XP:34:GLU:OE1   | 16:XP:55:ARG:HD3   | 2.10                     | 0.52              |
| 25:YA:184:C:H2'    | 25:YA:185:U:C6     | 2.45                     | 0.52              |
| 25:YA:1156:A:C8    | 40:YU:51:LYS:HD2   | 2.43                     | 0.52              |
| 25:YA:1292:U:H2'   | 25:YA:1293:C:C6    | 2.44                     | 0.52              |
| 33:YN:12:ARG:NH1   | 33:YN:50:ASP:OD1   | 2.43                     | 0.52              |
| 37:YR:53:HIS:HA    | 37:YR:56:LYS:HD3   | 1.90                     | 0.52              |
| 38:YS:25:ARG:HH11  | 38:YS:25:ARG:CB    | 2.22                     | 0.52              |
| 39:YT:23:ARG:HG2   | 39:YT:120:ARG:HH12 | 1.75                     | 0.52              |
| 42:YW:9:TYR:CD2    | 42:YW:102:HIS:HE1  | 2.28                     | 0.52              |
| 1:QA:1069:C:O2'    | 5:QE:25:ARG:NH1    | 2.42                     | 0.52              |
| 10:QJ:39:PRO:HB3   | 10:QJ:70:ARG:NH1   | 2.23                     | 0.52              |
| 14:QN:7:ILE:CG1    | 14:QN:8:GLU:N      | 2.72                     | 0.52              |
| 17:QQ:98:LEU:O     | 17:QQ:99:SER:C     | 2.53                     | 0.52              |
| 20:QT:28:ALA:C     | 20:QT:30:LYS:N     | 2.67                     | 0.52              |
| 20:QT:89:ARG:HH22  | 20:QT:106:ALA:HB2  | 1.75                     | 0.52              |
| 25:RA:103:A:OP2    | 25:RA:103:A:H8     | 1.92                     | 0.52              |
| 25:RA:1047:G:H2'   | 25:RA:1110:G:N1    | 2.24                     | 0.52              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:2198:A:HO2'   | 25:RA:2199:A:P     | 2.33                     | 0.52              |
| 25:RA:2319:G:N7     | 38:RS:3:ARG:HB3    | 2.25                     | 0.52              |
| 26:RB:43:C:C4       | 26:RB:45:A:C6      | 2.98                     | 0.52              |
| 27:RD:35:LYS:HG2    | 27:RD:64:ILE:HG22  | 1.92                     | 0.52              |
| 27:RD:133:LEU:HG    | 27:RD:189:CYS:O    | 2.10                     | 0.52              |
| 27:RD:165:ILE:C     | 27:RD:166:GLN:HE21 | 2.18                     | 0.52              |
| 28:RE:54:GLN:NE2    | 28:RE:54:GLN:H     | 2.08                     | 0.52              |
| 28:RE:129:HIS:O     | 28:RE:130:GLY:C    | 2.53                     | 0.52              |
| 28:RE:170:LEU:CD2   | 28:RE:185:LYS:HB2  | 2.40                     | 0.52              |
| 28:RE:179:GLU:HA    | 28:RE:179:GLU:OE1  | 2.10                     | 0.52              |
| 31:RH:4:ILE:O       | 31:RH:6:ARG:N      | 2.43                     | 0.52              |
| 38:RS:25:ARG:HH12   | 38:RS:42:ASP:CG    | 2.16                     | 0.52              |
| 39:RT:16:ARG:HD3    | 39:RT:19:LEU:HG    | 1.92                     | 0.52              |
| 39:RT:23:ARG:HG2    | 39:RT:120:ARG:HH12 | 1.75                     | 0.52              |
| 39:RT:94:ALA:O      | 39:RT:95:ARG:HB3   | 2.09                     | 0.52              |
| 41:RV:3:ALA:HB3     | 41:RV:14:VAL:HG23  | 1.92                     | 0.52              |
| 49:R3:6:VAL:HG12    | 49:R3:56:VAL:HG22  | 1.91                     | 0.52              |
| 50:R4:54:GLY:HA2    | 50:R4:57:GLU:HG2   | 1.92                     | 0.52              |
| 1:XA:607:A:C2       | 16:XP:31:LYS:HB2   | 2.45                     | 0.52              |
| 2:XB:200:ILE:HG22   | 2:XB:201:ILE:N     | 2.24                     | 0.52              |
| 3:XC:140:ARG:HG3    | 3:XC:140:ARG:HH11  | 1.75                     | 0.52              |
| 4:XD:155:LEU:O      | 4:XD:159:ARG:HG2   | 2.10                     | 0.52              |
| 8:XH:102:ARG:NH1    | 8:XH:105:ARG:HH22  | 2.07                     | 0.52              |
| 9:XI:3:GLN:HB3      | 9:XI:20:ARG:CG     | 2.40                     | 0.52              |
| 15:XO:26:GLU:OE2    | 15:XO:77:ARG:NH1   | 2.43                     | 0.52              |
| 16:XP:45:THR:HG23   | 16:XP:46:PRO:CD    | 2.40                     | 0.52              |
| 18:XR:44:LEU:HD12   | 18:XR:44:LEU:N     | 2.24                     | 0.52              |
| 20:XT:83:ARG:O      | 20:XT:86:ARG:HB3   | 2.09                     | 0.52              |
| 25:YA:242:G:C8      | 54:Y8:5:LYS:HG2    | 2.44                     | 0.52              |
| 25:YA:270(T):G:H5'' | 47:Y1:97:LEU:CD2   | 2.30                     | 0.52              |
| 25:YA:1826:G:OP1    | 27:YD:224:ALA:N    | 2.35                     | 0.52              |
| 25:YA:2277:G:OP1    | 36:YQ:85:LYS:HB2   | 2.10                     | 0.52              |
| 28:YE:176:ILE:HG22  | 28:YE:176:ILE:O    | 2.10                     | 0.52              |
| 34:YO:2:ILE:CD1     | 34:YO:82:ASN:HD22  | 2.14                     | 0.52              |
| 34:YO:43:VAL:HG23   | 34:YO:56:ASP:O     | 2.10                     | 0.52              |
| 34:YO:113:LYS:HG2   | 34:YO:117:LEU:CD1  | 2.38                     | 0.52              |
| 38:YS:56:LEU:O      | 38:YS:57:LYS:C     | 2.53                     | 0.52              |
| 39:YT:42:ILE:HD12   | 39:YT:42:ILE:N     | 2.25                     | 0.52              |
| 39:YT:99:LEU:HB2    | 39:YT:101:PHE:CE1  | 2.45                     | 0.52              |
| 1:QA:1186:G:O3'     | 9:QI:113:LYS:NZ    | 2.35                     | 0.52              |
| 1:QA:1266:G:N2      | 1:QA:1269:A:OP2    | 2.39                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:232:PRO:O     | 2:QB:233:SER:O     | 2.27                     | 0.52              |
| 6:QF:10:LEU:HD13   | 6:QF:61:LEU:HD11   | 1.92                     | 0.52              |
| 7:QG:85:TYR:HE1    | 7:QG:154:TYR:HE1   | 1.56                     | 0.52              |
| 9:QI:13:ALA:HB2    | 9:QI:68:GLY:HA3    | 1.92                     | 0.52              |
| 10:QJ:81:THR:C     | 10:QJ:83:GLU:N     | 2.64                     | 0.52              |
| 11:QK:115:PRO:C    | 11:QK:117:ASN:H    | 2.17                     | 0.52              |
| 12:QL:32:PHE:HE1   | 12:QL:86:ARG:HG3   | 1.73                     | 0.52              |
| 13:QM:34:LEU:HD12  | 13:QM:41:PRO:HG3   | 1.92                     | 0.52              |
| 13:QM:77:ASN:CG    | 50:R4:71:ARG:NH1   | 2.68                     | 0.52              |
| 13:QM:81:LEU:HD13  | 13:QM:88:ARG:HD2   | 1.91                     | 0.52              |
| 14:QN:36:PHE:C     | 14:QN:36:PHE:CD1   | 2.88                     | 0.52              |
| 25:RA:153:C:P      | 47:R1:88:LYS:HE2   | 2.50                     | 0.52              |
| 25:RA:796:C:H2'    | 25:RA:797:C:C6     | 2.45                     | 0.52              |
| 25:RA:1803:A:N1    | 25:RA:1822:G:O2'   | 2.41                     | 0.52              |
| 25:RA:2331:G:H4'   | 46:R0:43:THR:H     | 1.75                     | 0.52              |
| 28:RE:54:GLN:O     | 28:RE:55:ASN:HB2   | 2.09                     | 0.52              |
| 28:RE:116:VAL:HG22 | 28:RE:122:PHE:HB2  | 1.91                     | 0.52              |
| 30:RG:97:ASP:N     | 30:RG:100:TRP:HD1  | 2.05                     | 0.52              |
| 32:RI:73:GLU:HG3   | 32:RI:136:VAL:HG23 | 1.92                     | 0.52              |
| 34:RO:4:PRO:O      | 34:RO:5:GLN:CB     | 2.58                     | 0.52              |
| 40:RU:92:ARG:NH2   | 40:RU:94:ASN:HD22  | 2.07                     | 0.52              |
| 41:RV:2:PHE:CD1    | 41:RV:2:PHE:C      | 2.88                     | 0.52              |
| 46:R0:68:GLU:OE1   | 46:R0:82:ARG:NH1   | 2.42                     | 0.52              |
| 49:R3:7:LYS:HE2    | 49:R3:32:GLN:NE2   | 2.25                     | 0.52              |
| 52:R6:30:THR:O     | 52:R6:30:THR:HG23  | 2.09                     | 0.52              |
| 55:R9:27:CYS:SG    | 55:R9:28:GLU:N     | 2.83                     | 0.52              |
| 1:XA:280:C:C2      | 17:XQ:38:ARG:HG3   | 2.43                     | 0.52              |
| 1:XA:411:A:C8      | 1:XA:413:G:H1'     | 2.45                     | 0.52              |
| 2:XB:170:GLU:HA    | 2:XB:172:ILE:CD1   | 2.40                     | 0.52              |
| 4:XD:65:ARG:NH1    | 4:XD:70:ILE:O      | 2.43                     | 0.52              |
| 6:XF:19:LEU:HD23   | 6:XF:19:LEU:C      | 2.35                     | 0.52              |
| 11:XK:46:GLY:HA2   | 11:XK:50:TYR:O     | 2.10                     | 0.52              |
| 11:XK:102:GLY:O    | 11:XK:103:LEU:C    | 2.53                     | 0.52              |
| 12:XL:127:GLU:O    | 12:XL:128:ALA:HB3  | 2.10                     | 0.52              |
| 13:XM:34:LEU:HD12  | 13:XM:41:PRO:HG3   | 1.92                     | 0.52              |
| 13:XM:92:HIS:CD2   | 13:XM:98:VAL:HG21  | 2.43                     | 0.52              |
| 13:XM:98:VAL:O     | 13:XM:98:VAL:HG12  | 2.10                     | 0.52              |
| 16:XP:1:MET:SD     | 16:XP:3:LYS:HE3    | 2.49                     | 0.52              |
| 19:XS:15:LEU:HD23  | 19:XS:15:LEU:H     | 1.74                     | 0.52              |
| 25:YA:287:C:H2'    | 25:YA:288:C:C6     | 2.44                     | 0.52              |
| 25:YA:680:G:H2'    | 25:YA:681:G:C8     | 2.44                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2159:G:H2'  | 25:YA:2160:G:C8    | 2.44                     | 0.52              |
| 25:YA:2392:A:H8   | 35:YP:60:MET:HG3   | 1.74                     | 0.52              |
| 25:YA:2734:A:H5'  | 25:YA:2735:G:OP2   | 2.09                     | 0.52              |
| 26:YB:41:U:C4     | 30:YG:70:VAL:HG23  | 2.45                     | 0.52              |
| 27:YD:133:LEU:HG  | 27:YD:189:CYS:O    | 2.10                     | 0.52              |
| 27:YD:174:ILE:N   | 27:YD:174:ILE:CD1  | 2.73                     | 0.52              |
| 29:YF:29:ASN:H    | 29:YF:112:MET:HE3  | 1.75                     | 0.52              |
| 29:YF:108:LYS:O   | 29:YF:112:MET:HG3  | 2.10                     | 0.52              |
| 38:YS:83:LYS:O    | 38:YS:109:GLY:CA   | 2.46                     | 0.52              |
| 38:YS:106:ARG:HA  | 38:YS:110:LEU:CG   | 2.39                     | 0.52              |
| 47:Y1:83:GLU:CG   | 47:Y1:84:GLY:N     | 2.71                     | 0.52              |
| 50:Y4:55:ARG:C    | 50:Y4:59:PHE:HB3   | 2.35                     | 0.52              |
| 54:Y8:43:GLN:C    | 54:Y8:44:LYS:HD2   | 2.35                     | 0.52              |
| 1:QA:376:G:H5''   | 16:QP:5:ARG:HD2    | 1.91                     | 0.52              |
| 1:QA:1055:A:O2'   | 3:QC:161:GLU:OE2   | 2.15                     | 0.52              |
| 1:QA:1151:A:H2'   | 1:QA:1152:A:C8     | 2.43                     | 0.52              |
| 1:QA:1343:G:H2'   | 1:QA:1344:C:C6     | 2.45                     | 0.52              |
| 2:QB:92:TYR:CE1   | 2:QB:151:GLY:HA3   | 2.45                     | 0.52              |
| 3:QC:6:HIS:C      | 3:QC:8:ILE:H       | 2.18                     | 0.52              |
| 3:QC:22:TRP:CZ3   | 3:QC:32:LEU:HD12   | 2.45                     | 0.52              |
| 4:QD:29:PRO:CG    | 4:QD:30:LYS:NZ     | 2.73                     | 0.52              |
| 4:QD:173:TRP:C    | 4:QD:186:LEU:HB2   | 2.35                     | 0.52              |
| 6:QF:99:ALA:HB1   | 18:QR:23:LYS:NZ    | 2.25                     | 0.52              |
| 7:QG:106:GLN:O    | 7:QG:110:GLN:HG3   | 2.10                     | 0.52              |
| 9:QI:112:LYS:HD3  | 9:QI:112:LYS:C     | 2.35                     | 0.52              |
| 13:QM:66:LEU:O    | 13:QM:68:GLY:N     | 2.43                     | 0.52              |
| 16:QP:40:ASP:C    | 16:QP:42:ARG:H     | 2.17                     | 0.52              |
| 19:QS:63:THR:O    | 19:QS:66:MET:HG2   | 2.09                     | 0.52              |
| 25:RA:704:G:H1'   | 25:RA:727:A:N6     | 2.25                     | 0.52              |
| 25:RA:2795:G:H3'  | 25:RA:2797:U:C5'   | 2.40                     | 0.52              |
| 26:RB:42:C:H42    | 30:RG:91:ARG:HH21  | 1.57                     | 0.52              |
| 27:RD:35:LYS:HD3  | 27:RD:63:ARG:CA    | 2.40                     | 0.52              |
| 27:RD:174:ILE:N   | 27:RD:174:ILE:CD1  | 2.73                     | 0.52              |
| 27:RD:198:ASN:C   | 27:RD:198:ASN:HD22 | 2.17                     | 0.52              |
| 33:RN:57:ALA:O    | 33:RN:58:ASP:HB3   | 2.09                     | 0.52              |
| 35:RP:88:LEU:HD23 | 35:RP:89:ALA:N     | 2.24                     | 0.52              |
| 35:RP:147:LEU:O   | 35:RP:148:LEU:CB   | 2.57                     | 0.52              |
| 47:R1:4:VAL:HG22  | 47:R1:5:CYS:N      | 2.25                     | 0.52              |
| 47:R1:76:ARG:HG2  | 47:R1:76:ARG:NH1   | 2.19                     | 0.52              |
| 48:R2:9:GLN:O     | 48:R2:12:GLU:HB3   | 2.10                     | 0.52              |
| 1:XA:642:A:N3     | 8:XH:113:SER:OG    | 2.33                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1054:C:P     | 1:XA:1197:G:OP2    | 2.67                     | 0.52              |
| 1:XA:1306:A:H61   | 1:XA:1331:G:H1'    | 1.75                     | 0.52              |
| 2:XB:53:ARG:O     | 2:XB:56:ARG:HB2    | 2.10                     | 0.52              |
| 2:XB:80:ILE:HD11  | 2:XB:208:ILE:CG2   | 2.23                     | 0.52              |
| 3:XC:112:SER:HB3  | 3:XC:115:LEU:HD12  | 1.92                     | 0.52              |
| 4:XD:26:CYS:HB3   | 4:XD:31:CYS:SG     | 2.49                     | 0.52              |
| 19:XS:3:ARG:HG3   | 19:XS:4:SER:N      | 2.24                     | 0.52              |
| 25:YA:2015:A:N3   | 51:Y5:2:ALA:N      | 2.58                     | 0.52              |
| 25:YA:2415:G:O3'  | 35:YP:66:GLY:HA3   | 2.10                     | 0.52              |
| 26:YB:42:C:H42    | 30:YG:91:ARG:NH2   | 2.05                     | 0.52              |
| 27:YD:35:LYS:HG2  | 27:YD:64:ILE:HG22  | 1.92                     | 0.52              |
| 27:YD:165:ILE:C   | 27:YD:166:GLN:HE21 | 2.18                     | 0.52              |
| 28:YE:61:ARG:O    | 28:YE:63:LEU:N     | 2.42                     | 0.52              |
| 28:YE:170:LEU:CD2 | 28:YE:185:LYS:HB2  | 2.40                     | 0.52              |
| 32:YI:88:ILE:HG12 | 32:YI:122:GLU:N    | 2.25                     | 0.52              |
| 33:YN:7:LYS:HD3   | 33:YN:9:VAL:N      | 2.25                     | 0.52              |
| 37:YR:41:ALA:O    | 37:YR:43:GLU:N     | 2.43                     | 0.52              |
| 39:YT:16:ARG:HD3  | 39:YT:19:LEU:HG    | 1.92                     | 0.52              |
| 40:YU:107:ALA:O   | 40:YU:111:GLU:OE1  | 2.28                     | 0.52              |
| 41:YV:48:GLY:O    | 41:YV:49:THR:C     | 2.52                     | 0.52              |
| 43:YX:52:VAL:HG12 | 43:YX:52:VAL:O     | 2.09                     | 0.52              |
| 44:YY:9:LYS:HG2   | 44:YY:9:LYS:O      | 2.10                     | 0.52              |
| 51:Y5:55:ARG:HG3  | 51:Y5:57:VAL:H     | 1.74                     | 0.52              |
| 1:QA:999:U:H2'    | 1:QA:1000:A:C8     | 2.45                     | 0.52              |
| 1:QA:1348:U:H4'   | 9:QI:120:ARG:HD2   | 1.91                     | 0.52              |
| 2:QB:53:ARG:O     | 2:QB:56:ARG:HB2    | 2.10                     | 0.52              |
| 3:QC:195:VAL:HG12 | 3:QC:196:LEU:H     | 1.75                     | 0.52              |
| 4:QD:65:ARG:NH1   | 4:QD:70:ILE:O      | 2.43                     | 0.52              |
| 4:QD:135:LEU:C    | 4:QD:137:SER:H     | 2.18                     | 0.52              |
| 4:QD:196:LEU:C    | 4:QD:198:VAL:N     | 2.66                     | 0.52              |
| 6:QF:19:LEU:HD23  | 6:QF:19:LEU:C      | 2.35                     | 0.52              |
| 25:RA:2637:U:H5'' | 28:RE:82:ARG:NH2   | 2.24                     | 0.52              |
| 29:RF:108:LYS:O   | 29:RF:112:MET:HG3  | 2.10                     | 0.52              |
| 34:RO:23:ARG:O    | 34:RO:39:ILE:HB    | 2.10                     | 0.52              |
| 37:RR:41:ALA:O    | 37:RR:43:GLU:N     | 2.43                     | 0.52              |
| 40:RU:107:ALA:O   | 40:RU:111:GLU:OE1  | 2.28                     | 0.52              |
| 42:RW:28:SER:HB3  | 42:RW:31:GLU:HB2   | 1.91                     | 0.52              |
| 43:RX:52:VAL:O    | 43:RX:52:VAL:HG12  | 2.09                     | 0.52              |
| 44:RY:91:GLU:HG3  | 44:RY:92:ASN:N     | 2.25                     | 0.52              |
| 55:R9:1:MET:HE1   | 55:R9:32:HIS:HD2   | 1.75                     | 0.52              |
| 1:XA:1322:C:O2'   | 1:XA:1323:G:H5'    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:XC:22:TRP:CZ3   | 3:XC:32:LEU:HD12   | 2.45                     | 0.52              |
| 3:XC:175:LEU:HD12 | 3:XC:175:LEU:H     | 1.75                     | 0.52              |
| 4:XD:106:TYR:CE1  | 4:XD:112:VAL:O     | 2.62                     | 0.52              |
| 4:XD:162:LEU:HD13 | 4:XD:181:MET:HB3   | 1.92                     | 0.52              |
| 8:XH:51:VAL:HG11  | 8:XH:60:ARG:HG3    | 1.92                     | 0.52              |
| 17:XQ:98:LEU:O    | 17:XQ:99:SER:C     | 2.53                     | 0.52              |
| 25:YA:242:G:H5'   | 54:Y8:62:LEU:CD2   | 2.38                     | 0.52              |
| 25:YA:558:G:OP1   | 33:YN:111:PRO:HD2  | 2.10                     | 0.52              |
| 25:YA:2372:G:H4'  | 52:Y6:46:HIS:CD2   | 2.45                     | 0.52              |
| 25:YA:2540:C:H2'  | 25:YA:2541:A:O4'   | 2.10                     | 0.52              |
| 27:YD:43:ARG:NH1  | 27:YD:44:ASN:OD1   | 2.42                     | 0.52              |
| 27:YD:205:VAL:O   | 27:YD:206:LEU:C    | 2.52                     | 0.52              |
| 28:YE:54:GLN:O    | 28:YE:55:ASN:HB2   | 2.09                     | 0.52              |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA2  | 1.91                     | 0.52              |
| 33:YN:94:HIS:O    | 33:YN:95:PRO:O     | 2.27                     | 0.52              |
| 34:YO:16:ALA:HA   | 34:YO:46:ALA:HB2   | 1.92                     | 0.52              |
| 39:YT:111:ARG:O   | 39:YT:112:ARG:CG   | 2.55                     | 0.52              |
| 40:YU:59:ARG:O    | 40:YU:63:VAL:HG23  | 2.10                     | 0.52              |
| 44:YY:74:PRO:O    | 44:YY:80:GLY:HA2   | 2.10                     | 0.52              |
| 47:Y1:91:LYS:HE3  | 47:Y1:91:LYS:CA    | 2.40                     | 0.52              |
| 52:Y6:34:LEU:HD23 | 52:Y6:36:LEU:HD22  | 1.92                     | 0.52              |
| 1:QA:411:A:N6     | 1:QA:413:G:H21     | 2.06                     | 0.51              |
| 1:QA:940:C:H2'    | 1:QA:941:G:C8      | 2.44                     | 0.51              |
| 3:QC:11:ARG:O     | 3:QC:13:GLY:N      | 2.43                     | 0.51              |
| 3:QC:35:GLU:OE2   | 3:QC:95:THR:HG23   | 2.10                     | 0.51              |
| 3:QC:150:LYS:HG3  | 3:QC:169:ALA:HB2   | 1.92                     | 0.51              |
| 5:QE:96:PRO:HA    | 5:QE:117:ASP:CG    | 2.35                     | 0.51              |
| 6:QF:10:LEU:HD13  | 6:QF:61:LEU:HD13   | 1.92                     | 0.51              |
| 6:QF:75:LEU:HD21  | 6:QF:79:LEU:HD11   | 1.91                     | 0.51              |
| 15:QO:16:ALA:HB1  | 15:QO:21:ASP:HB3   | 1.92                     | 0.51              |
| 18:QR:64:ARG:O    | 18:QR:66:LEU:N     | 2.43                     | 0.51              |
| 19:QS:40:ILE:HG23 | 19:QS:67:VAL:O     | 2.11                     | 0.51              |
| 25:RA:923:C:H2'   | 25:RA:924:C:C6     | 2.44                     | 0.51              |
| 26:RB:3:C:H2'     | 26:RB:4:C:C6       | 2.45                     | 0.51              |
| 28:RE:93:VAL:C    | 28:RE:95:ILE:H     | 2.17                     | 0.51              |
| 28:RE:105:THR:HB  | 28:RE:197:ILE:HG12 | 1.92                     | 0.51              |
| 30:RG:97:ASP:O    | 30:RG:101:ILE:HG23 | 2.10                     | 0.51              |
| 31:RH:24:VAL:O    | 31:RH:24:VAL:HG23  | 2.10                     | 0.51              |
| 31:RH:126:PRO:HD2 | 31:RH:127:GLU:N    | 2.25                     | 0.51              |
| 33:RN:16:ILE:HG22 | 33:RN:17:ASP:N     | 2.26                     | 0.51              |
| 34:RO:2:ILE:HD12  | 34:RO:2:ILE:N      | 2.24                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:RR:52:ILE:CG2   | 37:RR:94:TYR:HD1   | 2.22                     | 0.51              |
| 40:RU:59:ARG:O     | 40:RU:63:VAL:HG23  | 2.10                     | 0.51              |
| 43:RX:47:PHE:N     | 43:RX:47:PHE:CD1   | 2.78                     | 0.51              |
| 43:RX:65:ARG:H     | 43:RX:65:ARG:CD    | 2.23                     | 0.51              |
| 50:R4:14:ILE:HG23  | 50:R4:14:ILE:O     | 2.10                     | 0.51              |
| 50:R4:40:HIS:N     | 50:R4:41:PRO:CD    | 2.73                     | 0.51              |
| 1:XA:186:C:H2'     | 1:XA:186(A):C:C6   | 2.45                     | 0.51              |
| 2:XB:5:ILE:N       | 2:XB:5:ILE:HD13    | 2.25                     | 0.51              |
| 2:XB:92:TYR:CD1    | 2:XB:92:TYR:C      | 2.88                     | 0.51              |
| 4:XD:162:LEU:HD11  | 4:XD:181:MET:HB3   | 1.92                     | 0.51              |
| 4:XD:173:TRP:C     | 4:XD:186:LEU:HB2   | 2.36                     | 0.51              |
| 5:XE:101:ILE:N     | 5:XE:101:ILE:HD13  | 2.25                     | 0.51              |
| 6:XF:30:LEU:O      | 6:XF:35:ALA:HB3    | 2.10                     | 0.51              |
| 6:XF:99:ALA:HB1    | 18:XR:23:LYS:NZ    | 2.25                     | 0.51              |
| 6:XF:101:ALA:HA    | 18:XR:28:GLU:OE1   | 2.10                     | 0.51              |
| 7:XG:16:LEU:HD11   | 9:XI:45:ALA:HB2    | 1.92                     | 0.51              |
| 7:XG:151:TYR:HA    | 7:XG:153:HIS:CE1   | 2.45                     | 0.51              |
| 13:XM:90:LEU:CB    | 13:XM:93:ARG:HD2   | 2.40                     | 0.51              |
| 14:XN:8:GLU:C      | 14:XN:10:ALA:N     | 2.68                     | 0.51              |
| 25:YA:755:C:H2'    | 25:YA:756:C:C6     | 2.46                     | 0.51              |
| 25:YA:2392:A:C8    | 35:YP:60:MET:HG3   | 2.45                     | 0.51              |
| 25:YA:2723:C:H5''  | 37:YR:1:MET:HG2    | 1.92                     | 0.51              |
| 27:YD:221:VAL:HG22 | 27:YD:226:MET:HE2  | 1.91                     | 0.51              |
| 29:YF:125:LEU:HA   | 29:YF:194:MET:O    | 2.10                     | 0.51              |
| 30:YG:97:ASP:O     | 30:YG:101:ILE:HG23 | 2.10                     | 0.51              |
| 33:YN:134:ARG:O    | 33:YN:136:GLU:N    | 2.43                     | 0.51              |
| 34:YO:14:THR:HG21  | 34:YO:86:ILE:HD13  | 1.91                     | 0.51              |
| 36:YQ:119:ARG:HG2  | 36:YQ:119:ARG:NH1  | 2.20                     | 0.51              |
| 38:YS:89:ARG:HG2   | 38:YS:89:ARG:HH11  | 1.74                     | 0.51              |
| 39:YT:110:ILE:HG23 | 39:YT:111:ARG:N    | 2.24                     | 0.51              |
| 40:YU:91:ASP:O     | 40:YU:92:ARG:C     | 2.53                     | 0.51              |
| 47:Y1:29:GLY:C     | 47:Y1:30:VAL:CG2   | 2.82                     | 0.51              |
| 2:QB:86:GLU:C      | 2:QB:88:ALA:H      | 2.16                     | 0.51              |
| 3:QC:40:ARG:O      | 3:QC:44:GLU:HG3    | 2.11                     | 0.51              |
| 3:QC:112:SER:HB3   | 3:QC:115:LEU:HD12  | 1.92                     | 0.51              |
| 4:QD:127:THR:CG2   | 4:QD:128:VAL:N     | 2.73                     | 0.51              |
| 5:QE:60:TYR:CE1    | 5:QE:64:ARG:NH2    | 2.77                     | 0.51              |
| 13:QM:2:ALA:O      | 13:QM:9:ILE:HB     | 2.10                     | 0.51              |
| 16:QP:21:VAL:O     | 16:QP:33:ILE:HG12  | 2.11                     | 0.51              |
| 25:RA:307:G:N2     | 25:RA:309:G:H3'    | 2.25                     | 0.51              |
| 25:RA:1204:A:O2'   | 25:RA:1205:U:O5'   | 2.28                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2439:A:C8    | 25:RA:2439:A:H5'   | 2.44                     | 0.51              |
| 25:RA:2868:A:H2'   | 25:RA:2869:G:C8    | 2.45                     | 0.51              |
| 27:RD:205:VAL:O    | 27:RD:206:LEU:C    | 2.52                     | 0.51              |
| 29:RF:162:LEU:HD23 | 29:RF:165:ARG:NH2  | 2.25                     | 0.51              |
| 29:RF:196:LEU:C    | 29:RF:197:ASP:O    | 2.50                     | 0.51              |
| 31:RH:55:PRO:HG2   | 31:RH:61:HIS:ND1   | 2.26                     | 0.51              |
| 33:RN:108:PRO:O    | 33:RN:113:GLY:HA3  | 2.10                     | 0.51              |
| 34:RO:24:VAL:HG21  | 34:RO:32:TYR:O     | 2.10                     | 0.51              |
| 34:RO:79:PHE:CD2   | 39:RT:72:VAL:HG22  | 2.44                     | 0.51              |
| 36:RQ:134:ARG:HH12 | 45:RZ:119:GLU:HG3  | 1.76                     | 0.51              |
| 39:RT:42:ILE:HD12  | 39:RT:42:ILE:N     | 2.24                     | 0.51              |
| 40:RU:8:VAL:O      | 40:RU:9:VAL:C      | 2.53                     | 0.51              |
| 44:RY:9:LYS:HG2    | 44:RY:9:LYS:O      | 2.10                     | 0.51              |
| 49:R3:17:LYS:HA    | 49:R3:20:LYS:HD2   | 1.93                     | 0.51              |
| 51:R5:20:ARG:C     | 51:R5:22:HIS:N     | 2.68                     | 0.51              |
| 51:R5:40:LYS:HD3   | 51:R5:46:CYS:SG    | 2.50                     | 0.51              |
| 1:XA:522:C:H41     | 12:XL:53:ARG:NH2   | 2.08                     | 0.51              |
| 1:XA:939:G:H5''    | 7:XG:102:ARG:NH1   | 2.25                     | 0.51              |
| 3:XC:20:SER:CB     | 3:XC:40:ARG:HH22   | 2.14                     | 0.51              |
| 3:XC:35:GLU:OE2    | 3:XC:95:THR:HG23   | 2.10                     | 0.51              |
| 3:XC:40:ARG:O      | 3:XC:44:GLU:HG3    | 2.11                     | 0.51              |
| 3:XC:181:ASN:HD21  | 3:XC:204:LEU:CD1   | 2.11                     | 0.51              |
| 4:XD:127:THR:CG2   | 4:XD:128:VAL:N     | 2.73                     | 0.51              |
| 6:XF:75:LEU:HD23   | 6:XF:79:LEU:HG     | 1.91                     | 0.51              |
| 9:XI:88:TYR:O      | 9:XI:89:ASN:CB     | 2.58                     | 0.51              |
| 11:XK:99:GLN:HE21  | 11:XK:105:VAL:HG21 | 1.76                     | 0.51              |
| 12:XL:23:LYS:O     | 12:XL:24:VAL:HG23  | 2.11                     | 0.51              |
| 13:XM:66:LEU:O     | 13:XM:68:GLY:N     | 2.43                     | 0.51              |
| 16:XP:21:VAL:O     | 16:XP:33:ILE:HG12  | 2.11                     | 0.51              |
| 25:YA:656:G:H2'    | 25:YA:657:U:O4'    | 2.11                     | 0.51              |
| 25:YA:753:C:O5'    | 25:YA:753:C:H6     | 1.93                     | 0.51              |
| 25:YA:841:A:H2'    | 25:YA:842:G:C8     | 2.46                     | 0.51              |
| 25:YA:1019:U:HO2'  | 25:YA:1021:A:H2    | 1.58                     | 0.51              |
| 25:YA:2815:C:H5'   | 51:Y5:29:THR:HG21  | 1.91                     | 0.51              |
| 27:YD:30:GLU:HG3   | 27:YD:63:ARG:NH2   | 2.25                     | 0.51              |
| 27:YD:35:LYS:HD2   | 27:YD:104:TYR:CD1  | 2.45                     | 0.51              |
| 28:YE:95:ILE:H     | 28:YE:95:ILE:CD1   | 2.19                     | 0.51              |
| 29:YF:65:TRP:HZ2   | 29:YF:72:ARG:NH2   | 2.08                     | 0.51              |
| 33:YN:12:ARG:NH1   | 33:YN:50:ASP:OD2   | 2.40                     | 0.51              |
| 34:YO:23:ARG:O     | 34:YO:39:ILE:HB    | 2.09                     | 0.51              |
| 35:YP:112:LEU:HD22 | 35:YP:113:LYS:H    | 1.75                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:67:ARG:HB2   | 38:YS:67:ARG:HH11 | 1.65                     | 0.51              |
| 41:YV:14:VAL:HA    | 41:YV:18:LEU:HD12 | 1.93                     | 0.51              |
| 44:YY:56:PRO:O     | 44:YY:57:GLN:C    | 2.53                     | 0.51              |
| 50:Y4:14:ILE:O     | 50:Y4:14:ILE:HG23 | 2.10                     | 0.51              |
| 50:Y4:68:ARG:HD3   | 50:Y4:69:LYS:HG2  | 1.92                     | 0.51              |
| 1:QA:595:G:H1'     | 1:QA:596:C:H5     | 1.75                     | 0.51              |
| 1:QA:959:A:O2'     | 1:QA:984:C:O2'    | 2.27                     | 0.51              |
| 1:QA:1177:G:OP2    | 9:QI:97:LYS:NZ    | 2.43                     | 0.51              |
| 2:QB:92:TYR:C      | 2:QB:92:TYR:CD1   | 2.88                     | 0.51              |
| 4:QD:196:LEU:HD12  | 4:QD:196:LEU:H    | 1.75                     | 0.51              |
| 6:QF:63:TYR:HD2    | 6:QF:63:TYR:N     | 2.09                     | 0.51              |
| 7:QG:15:ASP:CB     | 7:QG:20:ASP:H     | 2.13                     | 0.51              |
| 10:QJ:17:ASP:HA    | 10:QJ:20:ALA:HB3  | 1.93                     | 0.51              |
| 13:QM:87:TYR:C     | 13:QM:89:GLY:N    | 2.64                     | 0.51              |
| 13:QM:90:LEU:CB    | 13:QM:93:ARG:HD2  | 2.41                     | 0.51              |
| 13:QM:98:VAL:O     | 13:QM:98:VAL:HG12 | 2.10                     | 0.51              |
| 15:QO:61:GLY:C     | 15:QO:65:ARG:NH1  | 2.67                     | 0.51              |
| 25:RA:1090:U:H3    | 25:RA:1102:C:H1'  | 1.74                     | 0.51              |
| 25:RA:1336:A:H2'   | 25:RA:1337:G:C8   | 2.45                     | 0.51              |
| 25:RA:2734:A:H5'   | 25:RA:2735:G:OP2  | 2.10                     | 0.51              |
| 26:RB:55:U:C5'     | 30:RG:28:VAL:HG21 | 2.40                     | 0.51              |
| 29:RF:127:GLU:O    | 29:RF:129:PHE:N   | 2.39                     | 0.51              |
| 31:RH:89:ILE:O     | 31:RH:89:ILE:CG1  | 2.57                     | 0.51              |
| 33:RN:12:ARG:NH1   | 33:RN:50:ASP:OD1  | 2.43                     | 0.51              |
| 33:RN:131:GLN:CG   | 33:RN:132:ALA:H   | 2.20                     | 0.51              |
| 34:RO:43:VAL:HG23  | 34:RO:56:ASP:O    | 2.10                     | 0.51              |
| 35:RP:112:LEU:HD11 | 35:RP:114:ILE:CG2 | 2.40                     | 0.51              |
| 35:RP:112:LEU:HD22 | 35:RP:113:LYS:N   | 2.26                     | 0.51              |
| 36:RQ:64:ILE:HA    | 36:RQ:106:VAL:CG1 | 2.33                     | 0.51              |
| 37:RR:56:LYS:C     | 37:RR:58:GLY:H    | 2.18                     | 0.51              |
| 39:RT:20:PRO:HD2   | 39:RT:86:ILE:HG23 | 1.92                     | 0.51              |
| 39:RT:99:LEU:HB2   | 39:RT:101:PHE:CE1 | 2.45                     | 0.51              |
| 48:R2:15:LYS:H     | 48:R2:67:LYS:HE2  | 1.73                     | 0.51              |
| 50:R4:36:CYS:O     | 50:R4:39:CYS:CB   | 2.55                     | 0.51              |
| 1:XA:376:G:OP1     | 16:XP:5:ARG:HB2   | 2.11                     | 0.51              |
| 1:XA:974:A:OP2     | 14:XN:41:ARG:HG2  | 2.10                     | 0.51              |
| 2:XB:86:GLU:C      | 2:XB:88:ALA:H     | 2.17                     | 0.51              |
| 3:XC:11:ARG:O      | 3:XC:13:GLY:N     | 2.43                     | 0.51              |
| 3:XC:29:TYR:OH     | 14:XN:54:PRO:HD2  | 2.09                     | 0.51              |
| 4:XD:83:SER:HA     | 4:XD:89:THR:HG23  | 1.92                     | 0.51              |
| 4:XD:147:ALA:HA    | 4:XD:182:LYS:HA   | 1.91                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:XD:196:LEU:HD12  | 4:XD:196:LEU:H     | 1.75                     | 0.51              |
| 8:XH:12:ARG:NH1    | 8:XH:27:PRO:HD2    | 2.25                     | 0.51              |
| 13:XM:8:GLU:OE1    | 30:YG:115:ARG:NH2  | 2.43                     | 0.51              |
| 21:XU:3:LYS:HB3    | 21:XU:14:TRP:CD1   | 2.46                     | 0.51              |
| 25:YA:860:U:H1'    | 25:YA:2268:A:H5'   | 1.92                     | 0.51              |
| 25:YA:900:A:H5'    | 25:YA:901:A:OP2    | 2.10                     | 0.51              |
| 27:YD:67:PHE:CE1   | 27:YD:157:ARG:NH2  | 2.79                     | 0.51              |
| 28:YE:203:LYS:HE3  | 28:YE:204:ALA:CB   | 2.40                     | 0.51              |
| 30:YG:44:GLY:CA    | 30:YG:88:ILE:HD11  | 2.40                     | 0.51              |
| 41:YV:35:LEU:CD2   | 41:YV:57:VAL:HG22  | 2.32                     | 0.51              |
| 42:YW:14:PRO:O     | 42:YW:17:VAL:N     | 2.42                     | 0.51              |
| 48:Y2:15:LYS:H     | 48:Y2:67:LYS:HE2   | 1.73                     | 0.51              |
| 54:Y8:29:LYS:HB2   | 54:Y8:44:LYS:HG2   | 1.90                     | 0.51              |
| 1:QA:277:C:OP1     | 17:QQ:68:ARG:NH2   | 2.32                     | 0.51              |
| 1:QA:1326:C:H2'    | 1:QA:1327:C:C6     | 2.45                     | 0.51              |
| 3:QC:22:TRP:CH2    | 3:QC:32:LEU:HB2    | 2.45                     | 0.51              |
| 3:QC:36:ASP:HB3    | 3:QC:40:ARG:NH1    | 2.25                     | 0.51              |
| 7:QG:140:ASP:C     | 7:QG:142:GLU:N     | 2.68                     | 0.51              |
| 9:QI:126:SER:O     | 9:QI:128:ARG:N     | 2.35                     | 0.51              |
| 20:QT:83:ARG:O     | 20:QT:86:ARG:HB3   | 2.10                     | 0.51              |
| 25:RA:1062:G:H2'   | 25:RA:1063:G:C8    | 2.46                     | 0.51              |
| 25:RA:2477:C:H41   | 55:R9:10:ILE:HG23  | 1.76                     | 0.51              |
| 28:RE:105:THR:HG23 | 28:RE:166:THR:OG1  | 2.10                     | 0.51              |
| 30:RG:114:ILE:CG2  | 30:RG:115:ARG:N    | 2.73                     | 0.51              |
| 31:RH:41:MET:HE1   | 31:RH:64:LEU:HB3   | 1.91                     | 0.51              |
| 36:RQ:25:ASP:HA    | 36:RQ:100:GLY:O    | 2.11                     | 0.51              |
| 37:RR:28:LEU:CD2   | 37:RR:114:VAL:HG12 | 2.41                     | 0.51              |
| 39:RT:57:PHE:O     | 39:RT:58:ASN:C     | 2.53                     | 0.51              |
| 41:RV:29:PRO:O     | 41:RV:61:VAL:O     | 2.29                     | 0.51              |
| 42:RW:9:TYR:CD2    | 42:RW:102:HIS:HE1  | 2.28                     | 0.51              |
| 42:RW:25:ARG:HB2   | 42:RW:25:ARG:HH11  | 1.74                     | 0.51              |
| 43:RX:5:TYR:CE2    | 48:R2:30:ARG:HG3   | 2.45                     | 0.51              |
| 44:RY:61:ILE:HG23  | 44:RY:62:GLU:N     | 2.24                     | 0.51              |
| 1:XA:1397:C:O2'    | 1:XA:1398:A:OP1    | 2.27                     | 0.51              |
| 2:XB:134:GLU:HB3   | 2:XB:138:LEU:CD1   | 2.39                     | 0.51              |
| 3:XC:6:HIS:C       | 3:XC:8:ILE:H       | 2.18                     | 0.51              |
| 3:XC:22:TRP:CH2    | 3:XC:32:LEU:HB2    | 2.45                     | 0.51              |
| 3:XC:124:ILE:C     | 3:XC:126:ARG:H     | 2.19                     | 0.51              |
| 7:XG:15:ASP:CB     | 7:XG:20:ASP:H      | 2.13                     | 0.51              |
| 8:XH:33:GLU:C      | 8:XH:35:ILE:N      | 2.66                     | 0.51              |
| 8:XH:39:LEU:C      | 8:XH:45:ILE:HG12   | 2.35                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:XI:112:LYS:HD3   | 9:XI:112:LYS:C    | 2.35                     | 0.51              |
| 10:XJ:17:ASP:HA    | 10:XJ:20:ALA:HB3  | 1.93                     | 0.51              |
| 13:XM:4:ILE:HG22   | 13:XM:5:ALA:H     | 1.75                     | 0.51              |
| 14:YN:36:PHE:CD1   | 14:YN:36:PHE:C    | 2.88                     | 0.51              |
| 16:XP:13:HIS:C     | 16:XP:15:PRO:HD3  | 2.36                     | 0.51              |
| 19:XS:40:ILE:HG23  | 19:XS:67:VAL:O    | 2.11                     | 0.51              |
| 20:XT:89:ARG:HH22  | 20:XT:106:ALA:HB2 | 1.75                     | 0.51              |
| 22:XV:58:A:O2'     | 22:XV:60:U:OP2    | 2.16                     | 0.51              |
| 25:YA:414:C:H2'    | 25:YA:415:A:C8    | 2.46                     | 0.51              |
| 25:YA:924:C:H2'    | 25:YA:925:C:C6    | 2.45                     | 0.51              |
| 25:YA:2446:G:N2    | 25:YA:2449:U:O2   | 2.41                     | 0.51              |
| 27:YD:134:ARG:HB2  | 27:YD:135:PHE:HD2 | 1.75                     | 0.51              |
| 28:YE:20:ALA:C     | 28:YE:21:VAL:HG13 | 2.35                     | 0.51              |
| 30:YG:37:VAL:HG22  | 30:YG:159:VAL:CA  | 2.34                     | 0.51              |
| 34:YO:4:PRO:O      | 34:YO:5:GLN:CB    | 2.57                     | 0.51              |
| 35:YP:101:VAL:HA   | 35:YP:105:LEU:O   | 2.10                     | 0.51              |
| 35:YP:112:LEU:HD11 | 35:YP:114:ILE:CG2 | 2.40                     | 0.51              |
| 51:Y5:40:LYS:HD3   | 51:Y5:46:CYS:SG   | 2.50                     | 0.51              |
| 1:QA:164:U:H2'     | 1:QA:165:C:C6     | 2.45                     | 0.51              |
| 1:QA:1053:G:O6     | 1:QA:1199:U:H2'   | 2.11                     | 0.51              |
| 1:QA:1074:G:H4'    | 2:QB:104:ASN:HB2  | 1.91                     | 0.51              |
| 2:QB:24:TRP:CE3    | 2:QB:26:PRO:HA    | 2.45                     | 0.51              |
| 6:QF:30:LEU:O      | 6:QF:35:ALA:HB3   | 2.10                     | 0.51              |
| 9:QI:3:GLN:HB3     | 9:QI:20:ARG:CG    | 2.40                     | 0.51              |
| 11:QK:96:ARG:O     | 11:QK:97:ALA:C    | 2.54                     | 0.51              |
| 11:QK:102:GLY:O    | 11:QK:103:LEU:C   | 2.53                     | 0.51              |
| 19:QS:3:ARG:HG3    | 19:QS:4:SER:N     | 2.24                     | 0.51              |
| 25:RA:242:G:N2     | 25:RA:254:G:H2'   | 2.25                     | 0.51              |
| 25:RA:945:A:O2'    | 25:RA:946:G:H4'   | 2.11                     | 0.51              |
| 25:RA:1998:G:OP2   | 28:RE:136:ARG:NH2 | 2.37                     | 0.51              |
| 25:RA:2406:U:N3    | 35:RP:72:PRO:HB2  | 2.26                     | 0.51              |
| 25:RA:2527:C:H5''  | 55:R9:30:PRO:HB2  | 1.91                     | 0.51              |
| 25:RA:2543:G:H2'   | 25:RA:2544:G:C8   | 2.45                     | 0.51              |
| 29:RF:32:LEU:O     | 29:RF:36:VAL:HG23 | 2.11                     | 0.51              |
| 30:RG:44:GLY:CA    | 30:RG:88:ILE:HD11 | 2.40                     | 0.51              |
| 30:RG:95:ARG:O     | 30:RG:96:ARG:C    | 2.54                     | 0.51              |
| 33:RN:26:LEU:HG    | 33:RN:30:ILE:HD11 | 1.93                     | 0.51              |
| 35:RP:112:LEU:HD22 | 35:RP:113:LYS:H   | 1.75                     | 0.51              |
| 37:RR:117:VAL:CG2  | 37:RR:118:GLU:N   | 2.74                     | 0.51              |
| 38:RS:87:PHE:O     | 38:RS:88:ASP:O    | 2.29                     | 0.51              |
| 39:RT:111:ARG:C    | 39:RT:113:LYS:N   | 2.64                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:RV:38:LEU:HD13  | 41:RV:55:ALA:HB3   | 1.91                     | 0.51              |
| 42:RW:7:ALA:HB2    | 42:RW:50:VAL:CG2   | 2.39                     | 0.51              |
| 44:RY:75:ILE:CG1   | 44:RY:76:CYS:N     | 2.73                     | 0.51              |
| 47:R1:8:SER:HB3    | 47:R1:66:HIS:CE1   | 2.46                     | 0.51              |
| 49:R3:49:LYS:O     | 49:R3:49:LYS:HG2   | 2.10                     | 0.51              |
| 1:XA:971:G:H5''    | 1:XA:972:C:H5''    | 1.92                     | 0.51              |
| 1:XA:1318:A:H4'    | 19:XS:11:VAL:CG1   | 2.40                     | 0.51              |
| 2:XB:178:ARG:HH21  | 8:XH:74:PRO:CB     | 2.11                     | 0.51              |
| 11:XK:29:ILE:HG13  | 11:XK:44:SER:HB3   | 1.92                     | 0.51              |
| 12:XL:24:VAL:O     | 12:XL:24:VAL:CG1   | 2.58                     | 0.51              |
| 13:XM:87:TYR:C     | 13:XM:89:GLY:H     | 2.18                     | 0.51              |
| 18:XR:64:ARG:O     | 18:XR:66:LEU:N     | 2.43                     | 0.51              |
| 25:YA:92:G:H2'     | 25:YA:93:C:C6      | 2.45                     | 0.51              |
| 25:YA:573:G:O2'    | 25:YA:574:C:H3'    | 2.10                     | 0.51              |
| 25:YA:1266:G:C5    | 42:YW:15:ARG:NH1   | 2.78                     | 0.51              |
| 25:YA:1530:G:O6    | 25:YA:1542:G:N2    | 2.44                     | 0.51              |
| 25:YA:1794:U:H2'   | 25:YA:1795:C:H6    | 1.76                     | 0.51              |
| 25:YA:1858:G:O2'   | 25:YA:1884:A:N6    | 2.43                     | 0.51              |
| 30:YG:114:ILE:CG2  | 30:YG:115:ARG:N    | 2.73                     | 0.51              |
| 33:YN:120:LEU:CD1  | 33:YN:122:VAL:HG23 | 2.39                     | 0.51              |
| 35:YP:12:ALA:C     | 35:YP:14:LYS:H     | 2.16                     | 0.51              |
| 37:YR:56:LYS:C     | 37:YR:58:GLY:H     | 2.18                     | 0.51              |
| 39:YT:14:TYR:H     | 39:YT:14:TYR:HD1   | 1.56                     | 0.51              |
| 40:YU:98:LEU:HD23  | 40:YU:98:LEU:C     | 2.36                     | 0.51              |
| 41:YV:2:PHE:CD1    | 41:YV:2:PHE:C      | 2.88                     | 0.51              |
| 45:YZ:103:ARG:HB2  | 45:YZ:138:GLU:HG2  | 1.91                     | 0.51              |
| 50:Y4:42:PHE:O     | 50:Y4:44:THR:N     | 2.44                     | 0.51              |
| 54:Y8:52:LYS:N     | 54:Y8:53:PRO:HD2   | 2.22                     | 0.51              |
| 1:QA:45:U:H2'      | 1:QA:46:G:C8       | 2.46                     | 0.51              |
| 1:QA:157:G:H2'     | 1:QA:158:G:H8      | 1.75                     | 0.51              |
| 1:QA:1502:A:H2     | 1:QA:1505:G:H22    | 1.59                     | 0.51              |
| 2:QB:134:GLU:HB3   | 2:QB:138:LEU:HD12  | 1.93                     | 0.51              |
| 4:QD:54:TYR:CE1    | 4:QD:206:PHE:HE1   | 2.29                     | 0.51              |
| 4:QD:162:LEU:HD11  | 4:QD:181:MET:HB3   | 1.92                     | 0.51              |
| 8:QH:39:LEU:C      | 8:QH:45:ILE:HG12   | 2.35                     | 0.51              |
| 13:QM:16:ASP:HB3   | 13:QM:34:LEU:HD11  | 1.93                     | 0.51              |
| 15:QO:17:ARG:NH1   | 15:QO:77:ARG:NH1   | 2.59                     | 0.51              |
| 19:QS:15:LEU:HD23  | 19:QS:15:LEU:H     | 1.75                     | 0.51              |
| 21:QU:10:ARG:HH11  | 21:QU:10:ARG:HG3   | 1.76                     | 0.51              |
| 25:RA:270(R):G:H2' | 25:RA:270(S):G:H8  | 1.73                     | 0.51              |
| 25:RA:1309:G:H4'   | 53:R7:7:PRO:HB2    | 1.92                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1779:U:OP2   | 25:RA:1784:A:N6   | 2.37                     | 0.51              |
| 26:RB:43:C:N4      | 26:RB:45:A:C6     | 2.79                     | 0.51              |
| 26:RB:45:A:H1'     | 30:RG:95:ARG:NH2  | 2.25                     | 0.51              |
| 27:RD:67:PHE:CE1   | 27:RD:157:ARG:NH2 | 2.79                     | 0.51              |
| 27:RD:221:VAL:HG22 | 27:RD:226:MET:HE2 | 1.91                     | 0.51              |
| 28:RE:47:VAL:O     | 28:RE:48:GLN:C    | 2.51                     | 0.51              |
| 28:RE:119:ARG:HD3  | 28:RE:160:TYR:HB2 | 1.91                     | 0.51              |
| 34:RO:16:ALA:HA    | 34:RO:46:ALA:HB2  | 1.92                     | 0.51              |
| 39:RT:34:VAL:CG1   | 39:RT:36:GLU:HG2  | 2.39                     | 0.51              |
| 44:RY:95:LYS:O     | 44:RY:96:ILE:O    | 2.28                     | 0.51              |
| 45:RZ:8:TYR:HB2    | 45:RZ:38:TYR:CE2  | 2.46                     | 0.51              |
| 47:R1:94:LEU:O     | 47:R1:95:LEU:HG   | 2.11                     | 0.51              |
| 54:R8:10:ALA:O     | 54:R8:14:VAL:HG12 | 2.11                     | 0.51              |
| 1:XA:554:C:H2'     | 1:XA:555:C:H6     | 1.75                     | 0.51              |
| 1:XA:640:A:O2'     | 8:XH:115:SER:HB3  | 2.11                     | 0.51              |
| 1:XA:1502:A:H2'    | 1:XA:1504:G:N7    | 2.26                     | 0.51              |
| 3:XC:87:LEU:C      | 3:XC:89:GLU:N     | 2.65                     | 0.51              |
| 5:XE:10:MET:HE2    | 5:XE:13:ILE:CD1   | 2.41                     | 0.51              |
| 6:XF:10:LEU:HD13   | 6:XF:61:LEU:HD13  | 1.92                     | 0.51              |
| 7:XG:140:ASP:C     | 7:XG:142:GLU:N    | 2.69                     | 0.51              |
| 21:XU:6:ARG:HE     | 21:XU:15:ARG:NH2  | 2.09                     | 0.51              |
| 22:XV:4:G:HO2'     | 22:XV:5:G:H8      | 1.58                     | 0.51              |
| 25:YA:27:G:O2'     | 25:YA:28:A:H8     | 1.93                     | 0.51              |
| 25:YA:1676:A:H8    | 25:YA:1676:A:O5'  | 1.93                     | 0.51              |
| 28:YE:51:PHE:CD1   | 28:YE:52:LEU:N    | 2.76                     | 0.51              |
| 40:YU:8:VAL:O      | 40:YU:9:VAL:C     | 2.53                     | 0.51              |
| 42:YW:70:TYR:HD2   | 42:YW:70:TYR:N    | 2.06                     | 0.51              |
| 54:Y8:40:GLU:C     | 54:Y8:42:ARG:N    | 2.68                     | 0.51              |
| 55:Y9:1:MET:HE2    | 55:Y9:10:ILE:HD13 | 1.92                     | 0.51              |
| 2:QB:187:LEU:HD13  | 2:QB:187:LEU:O    | 2.11                     | 0.51              |
| 3:QC:21:ARG:CD     | 3:QC:21:ARG:N     | 2.74                     | 0.51              |
| 6:QF:86:ARG:O      | 6:QF:87:ARG:CG    | 2.50                     | 0.51              |
| 8:QH:102:ARG:NH1   | 8:QH:105:ARG:HH12 | 2.09                     | 0.51              |
| 9:QI:28:VAL:O      | 9:QI:29:ASN:C     | 2.53                     | 0.51              |
| 13:QM:57:ARG:HH11  | 13:QM:57:ARG:CB   | 2.14                     | 0.51              |
| 25:RA:503:A:H4'    | 25:RA:504:U:C5'   | 2.40                     | 0.51              |
| 33:RN:6:PRO:HG2    | 33:RN:43:THR:OG1  | 2.11                     | 0.51              |
| 33:RN:134:ARG:O    | 33:RN:136:GLU:N   | 2.43                     | 0.51              |
| 37:RR:85:PRO:C     | 37:RR:87:TYR:H    | 2.19                     | 0.51              |
| 39:RT:36:GLU:O     | 39:RT:37:GLY:C    | 2.53                     | 0.51              |
| 41:RV:5:VAL:HG22   | 41:RV:14:VAL:HG22 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1151:A:H2'   | 1:XA:1152:A:C8     | 2.46                     | 0.51              |
| 4:XD:112:VAL:HG12 | 4:XD:116:GLN:OE1   | 2.10                     | 0.51              |
| 4:XD:135:LEU:C    | 4:XD:137:SER:H     | 2.18                     | 0.51              |
| 5:XE:96:PRO:HA    | 5:XE:117:ASP:CG    | 2.35                     | 0.51              |
| 6:XF:22:GLU:CD    | 6:XF:82:ARG:HH21   | 2.18                     | 0.51              |
| 7:XG:108:ALA:C    | 7:XG:110:GLN:H     | 2.19                     | 0.51              |
| 8:XH:29:SER:CB    | 8:XH:32:LYS:HG3    | 2.28                     | 0.51              |
| 12:XL:126:LYS:C   | 12:XL:128:ALA:N    | 2.69                     | 0.51              |
| 13:XM:2:ALA:O     | 13:XM:9:ILE:HB     | 2.10                     | 0.51              |
| 14:XN:44:LEU:O    | 14:XN:48:ALA:N     | 2.41                     | 0.51              |
| 16:XP:30:GLY:O    | 16:XP:31:LYS:C     | 2.54                     | 0.51              |
| 19:XS:41:VAL:CG1  | 19:XS:45:VAL:N     | 2.74                     | 0.51              |
| 25:YA:275:G:N2    | 25:YA:276:A:H62    | 2.09                     | 0.51              |
| 25:YA:593:G:H2'   | 25:YA:594:U:H6     | 1.74                     | 0.51              |
| 25:YA:1799:G:O2'  | 27:YD:270:ILE:HD11 | 2.11                     | 0.51              |
| 25:YA:2074:U:H2'  | 25:YA:2075:U:C6    | 2.46                     | 0.51              |
| 25:YA:2319:G:N7   | 38:YS:3:ARG:HB3    | 2.26                     | 0.51              |
| 27:YD:210:GLY:O   | 27:YD:213:ARG:N    | 2.43                     | 0.51              |
| 30:YG:109:VAL:O   | 30:YG:113:ARG:HG3  | 2.10                     | 0.51              |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:CG2   | 2.41                     | 0.51              |
| 31:YH:41:MET:HE1  | 31:YH:64:LEU:HB3   | 1.91                     | 0.51              |
| 31:YH:55:PRO:HG2  | 31:YH:61:HIS:ND1   | 2.26                     | 0.51              |
| 35:YP:49:ARG:HE   | 54:Y8:59:LYS:HG2   | 1.76                     | 0.51              |
| 36:YQ:133:ARG:HG2 | 36:YQ:134:ARG:N    | 2.26                     | 0.51              |
| 37:YR:118:GLU:OXT | 37:YR:118:GLU:HG3  | 2.11                     | 0.51              |
| 39:YT:14:TYR:N    | 39:YT:14:TYR:CD1   | 2.77                     | 0.51              |
| 43:YX:36:LYS:HA   | 43:YX:39:ILE:HD12  | 1.91                     | 0.51              |
| 43:YX:47:PHE:CD1  | 43:YX:47:PHE:N     | 2.78                     | 0.51              |
| 2:QB:82:ARG:HA    | 2:QB:92:TYR:CE2    | 2.46                     | 0.51              |
| 3:QC:124:ILE:C    | 3:QC:126:ARG:H     | 2.19                     | 0.51              |
| 5:QE:101:ILE:N    | 5:QE:101:ILE:HD13  | 2.25                     | 0.51              |
| 9:QI:88:TYR:O     | 9:QI:89:ASN:CB     | 2.58                     | 0.51              |
| 10:QJ:54:PHE:O    | 10:QJ:55:LYS:HG3   | 2.11                     | 0.51              |
| 13:QM:87:TYR:C    | 13:QM:89:GLY:H     | 2.18                     | 0.51              |
| 18:QR:43:PHE:C    | 18:QR:51:LEU:HD12  | 2.36                     | 0.51              |
| 21:QU:3:LYS:HB3   | 21:QU:14:TRP:CD1   | 2.45                     | 0.51              |
| 25:RA:251:A:C5    | 25:RA:252:G:H1'    | 2.46                     | 0.51              |
| 25:RA:1114:G:H2'  | 25:RA:1115:G:C8    | 2.45                     | 0.51              |
| 25:RA:2188:C:H2'  | 25:RA:2189:U:O4'   | 2.10                     | 0.51              |
| 27:RD:76:PRO:HA   | 27:RD:118:VAL:HG23 | 1.93                     | 0.51              |
| 28:RE:20:ALA:C    | 28:RE:21:VAL:HG13  | 2.35                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:RF:65:TRP:HZ2   | 29:RF:72:ARG:NH2  | 2.08                     | 0.51              |
| 29:RF:132:VAL:O    | 29:RF:133:ASN:C   | 2.52                     | 0.51              |
| 33:RN:112:LEU:HD23 | 33:RN:113:GLY:N   | 2.26                     | 0.51              |
| 34:RO:113:LYS:O    | 34:RO:116:SER:HB3 | 2.11                     | 0.51              |
| 38:RS:56:LEU:O     | 38:RS:57:LYS:C    | 2.53                     | 0.51              |
| 38:RS:89:ARG:HD2   | 38:RS:89:ARG:O    | 2.11                     | 0.51              |
| 47:R1:87:PRO:O     | 47:R1:91:LYS:HB2  | 2.11                     | 0.51              |
| 50:R4:12:ALA:HB1   | 50:R4:30:GLU:H    | 1.76                     | 0.51              |
| 52:R6:9:LEU:HB3    | 52:R6:26:ASN:O    | 2.11                     | 0.51              |
| 53:R7:36:GLN:HG2   | 53:R7:36:GLN:O    | 2.10                     | 0.51              |
| 1:XA:266:G:O2'     | 1:XA:267:C:OP2    | 2.25                     | 0.51              |
| 1:XA:817:C:H1'     | 1:XA:819:A:H5''   | 1.91                     | 0.51              |
| 1:XA:1119:C:H2'    | 1:XA:1120:G:H8    | 1.75                     | 0.51              |
| 3:XC:21:ARG:CD     | 3:XC:21:ARG:N     | 2.74                     | 0.51              |
| 3:XC:70:VAL:CG1    | 3:XC:71:ALA:N     | 2.73                     | 0.51              |
| 3:XC:139:GLN:O     | 3:XC:143:GLU:HB2  | 2.11                     | 0.51              |
| 9:XI:40:LEU:C      | 9:XI:42:ARG:H     | 2.18                     | 0.51              |
| 16:XP:1:MET:O      | 16:XP:3:LYS:HG3   | 2.11                     | 0.51              |
| 16:XP:20:VAL:HG23  | 16:XP:34:GLU:O    | 2.11                     | 0.51              |
| 16:XP:39:TYR:OH    | 16:XP:41:PRO:HB3  | 2.11                     | 0.51              |
| 18:XR:43:PHE:C     | 18:XR:44:LEU:HD12 | 2.36                     | 0.51              |
| 20:XT:28:ALA:C     | 20:XT:30:LYS:N    | 2.67                     | 0.51              |
| 21:XU:10:ARG:HH11  | 21:XU:10:ARG:HG3  | 1.75                     | 0.51              |
| 22:XV:68:C:H2'     | 22:XV:69:C:H6     | 1.76                     | 0.51              |
| 25:YA:704:G:H2'    | 25:YA:726:G:N2    | 2.25                     | 0.51              |
| 25:YA:1006:C:H1'   | 33:YN:106:MET:HE3 | 1.91                     | 0.51              |
| 25:YA:2420:C:H6    | 25:YA:2420:C:O5'  | 1.92                     | 0.51              |
| 25:YA:2452:C:O4'   | 56:Z8:76:PPU:CB   | 2.59                     | 0.51              |
| 27:YD:28:GLU:OE1   | 27:YD:29:PRO:HD2  | 2.11                     | 0.51              |
| 27:YD:117:VAL:CG2  | 27:YD:128:GLY:C   | 2.84                     | 0.51              |
| 30:YG:51:ARG:HH11  | 30:YG:51:ARG:HB3  | 1.76                     | 0.51              |
| 33:YN:108:PRO:O    | 33:YN:113:GLY:HA3 | 2.10                     | 0.51              |
| 35:YP:95:VAL:HG13  | 35:YP:100:LEU:CD2 | 2.41                     | 0.51              |
| 36:YQ:7:MET:HE1    | 36:YQ:73:PRO:HG3  | 1.91                     | 0.51              |
| 36:YQ:58:PHE:HD1   | 36:YQ:58:PHE:O    | 1.94                     | 0.51              |
| 38:YS:95:HIS:CG    | 38:YS:96:GLY:N    | 2.77                     | 0.51              |
| 41:YV:41:GLY:N     | 41:YV:46:VAL:HG13 | 2.26                     | 0.51              |
| 43:YX:65:ARG:H     | 43:YX:65:ARG:CD   | 2.24                     | 0.51              |
| 45:YZ:95:PRO:HG2   | 45:YZ:127:LYS:HD3 | 1.93                     | 0.51              |
| 49:Y3:56:VAL:CG1   | 49:Y3:57:GLU:N    | 2.74                     | 0.51              |
| 52:Y6:20:ASN:O     | 52:Y6:21:TYR:CB   | 2.59                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:64:G:H4'     | 1:QA:65:U:O5'      | 2.11                     | 0.51              |
| 1:QA:1034:G:H2'   | 1:QA:1035:A:C8     | 2.45                     | 0.51              |
| 1:QA:1159:U:O2'   | 1:QA:1160:G:N7     | 2.44                     | 0.51              |
| 2:QB:82:ARG:HB3   | 2:QB:83:MET:HE2    | 1.91                     | 0.51              |
| 3:QC:175:LEU:HD12 | 3:QC:175:LEU:H     | 1.75                     | 0.51              |
| 4:QD:112:VAL:HG12 | 4:QD:116:GLN:OE1   | 2.11                     | 0.51              |
| 5:QE:10:MET:HE2   | 5:QE:13:ILE:CD1    | 2.41                     | 0.51              |
| 7:QG:16:LEU:HD11  | 9:QI:45:ALA:HB2    | 1.92                     | 0.51              |
| 8:QH:104:ARG:HD2  | 8:QH:138:TRP:CD2   | 2.46                     | 0.51              |
| 9:QI:40:LEU:C     | 9:QI:42:ARG:H      | 2.18                     | 0.51              |
| 9:QI:79:LEU:HD22  | 9:QI:101:PHE:O     | 2.11                     | 0.51              |
| 25:RA:1614:A:H62  | 42:RW:93:ALA:HB2   | 1.76                     | 0.51              |
| 25:RA:1827:C:O2'  | 25:RA:1970:A:N3    | 2.38                     | 0.51              |
| 27:RD:117:VAL:CG2 | 27:RD:128:GLY:C    | 2.84                     | 0.51              |
| 30:RG:51:ARG:HH11 | 30:RG:51:ARG:HB3   | 1.76                     | 0.51              |
| 31:RH:131:VAL:CG1 | 31:RH:132:ARG:N    | 2.74                     | 0.51              |
| 36:RQ:36:ALA:HB1  | 36:RQ:127:ILE:HD12 | 1.93                     | 0.51              |
| 44:RY:46:LYS:HE3  | 44:RY:63:LYS:HB3   | 1.93                     | 0.51              |
| 44:RY:56:PRO:O    | 44:RY:57:GLN:C     | 2.53                     | 0.51              |
| 48:R2:36:ARG:O    | 48:R2:40:SER:HB2   | 2.11                     | 0.51              |
| 54:R8:61:LEU:O    | 54:R8:62:LEU:CB    | 2.57                     | 0.51              |
| 1:XA:1329:A:H5'   | 13:XM:29:ARG:HG3   | 1.93                     | 0.51              |
| 2:XB:187:LEU:HD13 | 2:XB:187:LEU:O     | 2.11                     | 0.51              |
| 3:XC:87:LEU:C     | 3:XC:89:GLU:H      | 2.19                     | 0.51              |
| 3:XC:150:LYS:HG3  | 3:XC:169:ALA:HB2   | 1.92                     | 0.51              |
| 4:XD:206:PHE:CD2  | 4:XD:207:TYR:CD1   | 2.99                     | 0.51              |
| 6:XF:10:LEU:HD13  | 6:XF:61:LEU:HD11   | 1.92                     | 0.51              |
| 6:XF:63:TYR:CD2   | 6:XF:63:TYR:N      | 2.79                     | 0.51              |
| 8:XH:104:ARG:HD2  | 8:XH:138:TRP:CD2   | 2.45                     | 0.51              |
| 16:XP:72:ARG:HD3  | 16:XP:73:LEU:HD23  | 1.91                     | 0.51              |
| 22:XV:15:G:H22    | 22:XV:48:C:H42     | 1.57                     | 0.51              |
| 25:YA:222:A:H3'   | 25:YA:421:U:H5'    | 1.92                     | 0.51              |
| 25:YA:952:G:P     | 36:YQ:16:ARG:HH12  | 2.34                     | 0.51              |
| 25:YA:1728:G:H8   | 25:YA:1732:A:H62   | 1.59                     | 0.51              |
| 28:YE:37:ARG:HE   | 28:YE:37:ARG:N     | 2.09                     | 0.51              |
| 33:YN:16:ILE:HG22 | 33:YN:17:ASP:N     | 2.25                     | 0.51              |
| 33:YN:118:LYS:O   | 33:YN:120:LEU:N    | 2.43                     | 0.51              |
| 34:YO:24:VAL:O    | 34:YO:24:VAL:HG13  | 2.11                     | 0.51              |
| 34:YO:24:VAL:HG21 | 34:YO:32:TYR:O     | 2.11                     | 0.51              |
| 38:YS:83:LYS:HG2  | 38:YS:109:GLY:HA2  | 1.90                     | 0.51              |
| 39:YT:51:ARG:HG3  | 39:YT:98:LYS:HG3   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:YX:5:TYR:CE2    | 48:Y2:30:ARG:HG3  | 2.46                     | 0.51              |
| 48:Y2:36:ARG:O     | 48:Y2:40:SER:HB2  | 2.10                     | 0.51              |
| 49:Y3:49:LYS:HG2   | 49:Y3:49:LYS:O    | 2.10                     | 0.51              |
| 50:Y4:12:ALA:HB1   | 50:Y4:30:GLU:H    | 1.76                     | 0.51              |
| 50:Y4:54:GLY:HA2   | 50:Y4:57:GLU:HG2  | 1.92                     | 0.51              |
| 51:Y5:36:CYS:C     | 51:Y5:38:ALA:H    | 2.19                     | 0.51              |
| 51:Y5:54:GLY:O     | 51:Y5:55:ARG:C    | 2.54                     | 0.51              |
| 1:QA:1347:G:H22    | 1:QA:1374:A:P     | 2.33                     | 0.51              |
| 1:QA:1499:A:H1'    | 1:QA:1520:G:H5'   | 1.93                     | 0.51              |
| 2:QB:23:ARG:HH11   | 2:QB:23:ARG:HG2   | 1.76                     | 0.51              |
| 3:QC:48:TYR:O      | 3:QC:51:GLY:N     | 2.41                     | 0.51              |
| 4:QD:12:CYS:HA     | 4:QD:19:LEU:HD23  | 1.83                     | 0.51              |
| 4:QD:22:LYS:HB2    | 4:QD:26:CYS:CB    | 2.41                     | 0.51              |
| 4:QD:83:SER:HA     | 4:QD:89:THR:HG23  | 1.92                     | 0.51              |
| 5:QE:83:GLU:HG2    | 5:QE:88:LYS:CG    | 2.41                     | 0.51              |
| 6:QF:101:ALA:HA    | 18:QR:28:GLU:OE1  | 2.11                     | 0.51              |
| 11:QK:46:GLY:HA2   | 11:QK:50:TYR:O    | 2.10                     | 0.51              |
| 12:QL:10:LEU:CD1   | 17:QQ:32:TYR:CD2  | 2.94                     | 0.51              |
| 12:QL:126:LYS:C    | 12:QL:128:ALA:N   | 2.69                     | 0.51              |
| 16:QP:45:THR:HG23  | 16:QP:46:PRO:CD   | 2.39                     | 0.51              |
| 25:RA:551:G:H5'    | 25:RA:1220:A:H1'  | 1.93                     | 0.51              |
| 25:RA:1007:C:O3'   | 33:RN:108:PRO:HB3 | 2.10                     | 0.51              |
| 25:RA:1814:G:H4'   | 27:RD:51:VAL:HG21 | 1.93                     | 0.51              |
| 25:RA:1903:G:OP2   | 27:RD:241:PRO:HB2 | 2.11                     | 0.51              |
| 28:RE:37:ARG:HE    | 28:RE:37:ARG:N    | 2.09                     | 0.51              |
| 34:RO:15:GLY:O     | 34:RO:46:ALA:HB1  | 2.10                     | 0.51              |
| 34:RO:23:ARG:HH11  | 34:RO:23:ARG:HG2  | 1.76                     | 0.51              |
| 37:RR:1:MET:O      | 37:RR:2:ARG:CB    | 2.59                     | 0.51              |
| 40:RU:112:ARG:HH11 | 40:RU:112:ARG:HG2 | 1.76                     | 0.51              |
| 50:R4:42:PHE:O     | 50:R4:44:THR:N    | 2.44                     | 0.51              |
| 1:XA:281:G:H8      | 1:XA:281:G:OP2    | 1.94                     | 0.51              |
| 1:XA:953:G:H5'     | 1:XA:965:A:H61    | 1.76                     | 0.51              |
| 2:XB:15:VAL:H      | 2:XB:16:HIS:HD1   | 1.59                     | 0.51              |
| 2:XB:53:ARG:HA     | 2:XB:56:ARG:HG3   | 1.93                     | 0.51              |
| 3:XC:184:TYR:HA    | 3:XC:200:ALA:O    | 2.11                     | 0.51              |
| 4:XD:178:VAL:O     | 4:XD:180:GLY:N    | 2.44                     | 0.51              |
| 5:XE:126:ARG:HH11  | 5:XE:126:ARG:CG   | 2.21                     | 0.51              |
| 6:XF:63:TYR:HD2    | 6:XF:63:TYR:N     | 2.09                     | 0.51              |
| 9:XI:28:VAL:O      | 9:XI:29:ASN:C     | 2.53                     | 0.51              |
| 21:XU:14:TRP:CE3   | 21:XU:15:ARG:HD3  | 2.46                     | 0.51              |
| 25:YA:363(A):A:H2' | 25:YA:363(B):G:H8 | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:639:U:H2'   | 25:YA:640:C:C6    | 2.46                     | 0.51              |
| 25:YA:1190:G:H5'  | 35:YP:32:THR:HA   | 1.92                     | 0.51              |
| 25:YA:1252:G:N3   | 40:YU:33:ARG:HD2  | 2.26                     | 0.51              |
| 25:YA:1833:U:O2'  | 25:YA:1969:A:N1   | 2.35                     | 0.51              |
| 25:YA:2377:A:H2'  | 25:YA:2378:A:C8   | 2.46                     | 0.51              |
| 25:YA:2774:C:H2'  | 25:YA:2775:A:O4'  | 2.11                     | 0.51              |
| 30:YG:95:ARG:O    | 30:YG:96:ARG:C    | 2.53                     | 0.51              |
| 31:YH:4:ILE:O     | 31:YH:6:ARG:N     | 2.43                     | 0.51              |
| 31:YH:72:ILE:O    | 31:YH:75:ALA:HB3  | 2.11                     | 0.51              |
| 31:YH:126:PRO:HD2 | 31:YH:127:GLU:N   | 2.25                     | 0.51              |
| 33:YN:26:LEU:HG   | 33:YN:30:ILE:HD11 | 1.92                     | 0.51              |
| 35:YP:62:LEU:CD2  | 35:YP:62:LEU:H    | 2.19                     | 0.51              |
| 36:YQ:25:ASP:HA   | 36:YQ:100:GLY:O   | 2.11                     | 0.51              |
| 38:YS:74:ALA:O    | 38:YS:75:GLU:C    | 2.54                     | 0.51              |
| 39:YT:20:PRO:HD2  | 39:YT:86:ILE:HG23 | 1.92                     | 0.51              |
| 41:YV:5:VAL:HG22  | 41:YV:14:VAL:HG22 | 1.93                     | 0.51              |
| 42:YW:48:ALA:O    | 42:YW:49:LYS:C    | 2.53                     | 0.51              |
| 44:YY:95:LYS:O    | 44:YY:96:ILE:O    | 2.28                     | 0.51              |
| 49:Y3:7:LYS:HE2   | 49:Y3:32:GLN:NE2  | 2.25                     | 0.51              |
| 50:Y4:10:VAL:HG23 | 50:Y4:11:PRO:HD2  | 1.93                     | 0.51              |
| 51:Y5:56:LYS:HD2  | 51:Y5:56:LYS:N    | 2.13                     | 0.51              |
| 1:QA:375:U:C4'    | 16:QP:17:TYR:HE2  | 2.24                     | 0.50              |
| 1:QA:438:G:H4'    | 4:QD:123:HIS:CE1  | 2.46                     | 0.50              |
| 1:QA:486:U:H2'    | 1:QA:487:A:H8     | 1.76                     | 0.50              |
| 1:QA:617:G:H1     | 1:QA:623:C:H42    | 1.59                     | 0.50              |
| 1:QA:1376:U:P     | 7:QG:94:ARG:HH12  | 2.33                     | 0.50              |
| 3:QC:99:VAL:O     | 3:QC:99:VAL:HG23  | 2.11                     | 0.50              |
| 3:QC:132:ARG:O    | 3:QC:136:GLN:HB2  | 2.11                     | 0.50              |
| 4:QD:155:LEU:O    | 4:QD:159:ARG:HG2  | 2.10                     | 0.50              |
| 4:QD:206:PHE:CD2  | 4:QD:207:TYR:CD1  | 2.99                     | 0.50              |
| 5:QE:12:LEU:HD23  | 5:QE:13:ILE:H     | 1.76                     | 0.50              |
| 7:QG:23:VAL:O     | 7:QG:27:ILE:CD1   | 2.60                     | 0.50              |
| 9:QI:29:ASN:OD1   | 9:QI:64:THR:HA    | 2.11                     | 0.50              |
| 12:QL:23:LYS:O    | 12:QL:24:VAL:HG23 | 2.10                     | 0.50              |
| 16:QP:1:MET:O     | 16:QP:3:LYS:HG3   | 2.11                     | 0.50              |
| 19:QS:43:GLU:N    | 19:QS:43:GLU:OE2  | 2.44                     | 0.50              |
| 25:RA:185:U:H4'   | 25:RA:218:A:H4'   | 1.93                     | 0.50              |
| 25:RA:1149:G:H2'  | 25:RA:1150:C:C6   | 2.46                     | 0.50              |
| 25:RA:1291:C:H2'  | 25:RA:1292:U:C6   | 2.46                     | 0.50              |
| 25:RA:2224:G:H4'  | 25:RA:2226:C:C2   | 2.46                     | 0.50              |
| 26:RB:13:A:N1     | 26:RB:69:G:O2'    | 2.41                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:137:HIS:HB3  | 28:RE:138:PRO:CD   | 2.37                     | 0.50              |
| 29:RF:127:GLU:OE1  | 29:RF:127:GLU:HA   | 2.07                     | 0.50              |
| 33:RN:7:LYS:HD3    | 33:RN:9:VAL:N      | 2.25                     | 0.50              |
| 34:RO:2:ILE:CD1    | 34:RO:82:ASN:HD22  | 2.14                     | 0.50              |
| 34:RO:20:MET:HG2   | 34:RO:21:CYS:O     | 2.11                     | 0.50              |
| 36:RQ:23:GLY:O     | 36:RQ:24:GLY:C     | 2.54                     | 0.50              |
| 41:RV:14:VAL:HA    | 41:RV:18:LEU:HD12  | 1.92                     | 0.50              |
| 41:RV:35:LEU:CD2   | 41:RV:57:VAL:HG22  | 2.32                     | 0.50              |
| 1:XA:89:U:O2'      | 1:XA:90:C:OP1      | 2.25                     | 0.50              |
| 1:XA:532:A:H2      | 1:XA:1206:G:H21    | 1.59                     | 0.50              |
| 3:XC:99:VAL:O      | 3:XC:99:VAL:HG23   | 2.11                     | 0.50              |
| 9:XI:83:ARG:C      | 9:XI:86:VAL:HG12   | 2.36                     | 0.50              |
| 12:XL:126:LYS:HB2  | 12:XL:126:LYS:HZ2  | 1.74                     | 0.50              |
| 13:XM:65:LYS:CE    | 50:Y4:50:VAL:HG11  | 2.41                     | 0.50              |
| 13:XM:66:LEU:O     | 13:XM:70:LEU:HB2   | 2.11                     | 0.50              |
| 15:XO:16:ALA:HB1   | 15:XO:21:ASP:HB3   | 1.92                     | 0.50              |
| 25:YA:270(J):G:H2' | 25:YA:270(K):C:O4' | 2.11                     | 0.50              |
| 25:YA:483:A:H4'    | 44:YY:49:VAL:HG13  | 1.92                     | 0.50              |
| 25:YA:1169:G:H1    | 25:YA:1180:C:N4    | 2.09                     | 0.50              |
| 25:YA:1683:C:H2'   | 25:YA:1684:C:C6    | 2.45                     | 0.50              |
| 25:YA:2722:G:H4'   | 37:YR:4:LEU:HB2    | 1.93                     | 0.50              |
| 25:YA:2728:U:H2'   | 25:YA:2729:G:C8    | 2.47                     | 0.50              |
| 28:YE:54:GLN:NE2   | 28:YE:54:GLN:H     | 2.08                     | 0.50              |
| 28:YE:105:THR:HG23 | 28:YE:166:THR:OG1  | 2.10                     | 0.50              |
| 28:YE:116:VAL:HG22 | 28:YE:122:PHE:HB2  | 1.91                     | 0.50              |
| 28:YE:129:HIS:O    | 28:YE:130:GLY:C    | 2.53                     | 0.50              |
| 31:YH:103:LEU:CD1  | 31:YH:131:VAL:HG21 | 2.41                     | 0.50              |
| 33:YN:73:THR:HG22  | 33:YN:82:LEU:HD11  | 1.93                     | 0.50              |
| 35:YP:114:ILE:HD13 | 35:YP:125:VAL:CG2  | 2.41                     | 0.50              |
| 38:YS:26:LEU:CD2   | 38:YS:87:PHE:CD1   | 2.94                     | 0.50              |
| 38:YS:83:LYS:HG2   | 38:YS:109:GLY:H    | 1.76                     | 0.50              |
| 38:YS:86:ALA:O     | 38:YS:87:PHE:HB3   | 2.10                     | 0.50              |
| 38:YS:87:PHE:O     | 38:YS:88:ASP:O     | 2.29                     | 0.50              |
| 47:Y1:80:LEU:HB2   | 47:Y1:81:LYS:CE    | 2.41                     | 0.50              |
| 47:Y1:85:LEU:HA    | 47:Y1:87:PRO:HD2   | 1.91                     | 0.50              |
| 51:Y5:20:ARG:C     | 51:Y5:22:HIS:N     | 2.68                     | 0.50              |
| 1:QA:596:C:N4      | 1:QA:644:G:H1      | 2.09                     | 0.50              |
| 1:QA:922:G:H4'     | 5:QE:20:GLN:HA     | 1.93                     | 0.50              |
| 1:QA:1392:G:H2'    | 1:QA:1393:U:O4'    | 2.11                     | 0.50              |
| 4:QD:7:PRO:HB2     | 4:QD:10:ARG:HD2    | 1.92                     | 0.50              |
| 4:QD:180:GLY:O     | 4:QD:181:MET:C     | 2.54                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:QE:45:PHE:CD2    | 5:QE:47:LYS:HD2    | 2.47                     | 0.50              |
| 7:QG:50:ILE:HA     | 7:QG:54:THR:HG22   | 1.93                     | 0.50              |
| 8:QH:12:ARG:NH1    | 8:QH:27:PRO:HD2    | 2.25                     | 0.50              |
| 11:QK:91:ARG:HH22  | 18:QR:88:LYS:NZ    | 2.09                     | 0.50              |
| 13:QM:118:ALA:O    | 22:QV:28:C:O3'     | 2.30                     | 0.50              |
| 13:QM:120:LYS:O    | 13:QM:121:LYS:HB2  | 2.11                     | 0.50              |
| 15:QO:76:GLU:C     | 15:QO:78:TYR:N     | 2.69                     | 0.50              |
| 16:QP:20:VAL:HG23  | 16:QP:34:GLU:O     | 2.11                     | 0.50              |
| 16:QP:30:GLY:O     | 16:QP:31:LYS:C     | 2.54                     | 0.50              |
| 21:QU:14:TRP:CE3   | 21:QU:15:ARG:HD3   | 2.46                     | 0.50              |
| 27:RD:30:GLU:HG3   | 27:RD:63:ARG:NH2   | 2.25                     | 0.50              |
| 31:RH:72:ILE:O     | 31:RH:75:ALA:HB3   | 2.11                     | 0.50              |
| 34:RO:35:VAL:O     | 34:RO:35:VAL:HG23  | 2.11                     | 0.50              |
| 34:RO:47:ILE:CG1   | 34:RO:48:PRO:HD2   | 2.41                     | 0.50              |
| 34:RO:107:ARG:CA   | 34:RO:112:MET:HE1  | 2.39                     | 0.50              |
| 35:RP:95:VAL:HG13  | 35:RP:100:LEU:CD2  | 2.40                     | 0.50              |
| 38:RS:83:LYS:HG2   | 38:RS:109:GLY:H    | 1.76                     | 0.50              |
| 38:RS:89:ARG:O     | 38:RS:90:GLY:C     | 2.54                     | 0.50              |
| 39:RT:57:PHE:CG    | 39:RT:58:ASN:N     | 2.79                     | 0.50              |
| 42:RW:88:ARG:HB3   | 42:RW:92:ARG:CB    | 2.41                     | 0.50              |
| 44:RY:44:ILE:CG1   | 44:RY:45:VAL:H     | 2.25                     | 0.50              |
| 47:R1:91:LYS:HE3   | 47:R1:91:LYS:CA    | 2.40                     | 0.50              |
| 51:R5:37:LYS:O     | 51:R5:37:LYS:HD2   | 2.12                     | 0.50              |
| 1:XA:27:G:C4'      | 4:XD:209:ARG:HG3   | 2.35                     | 0.50              |
| 2:XB:82:ARG:HA     | 2:XB:92:TYR:CE2    | 2.45                     | 0.50              |
| 2:XB:103:THR:N     | 2:XB:180:LEU:HD11  | 2.26                     | 0.50              |
| 7:XG:40:ALA:O      | 7:XG:41:ARG:C      | 2.54                     | 0.50              |
| 15:XO:76:GLU:C     | 15:XO:78:TYR:N     | 2.68                     | 0.50              |
| 18:XR:43:PHE:C     | 18:XR:51:LEU:HD12  | 2.36                     | 0.50              |
| 25:YA:357:A:H2'    | 25:YA:358:U:H6     | 1.76                     | 0.50              |
| 25:YA:669:G:H2'    | 25:YA:669:G:N3     | 2.24                     | 0.50              |
| 25:YA:2146:C:H4'   | 25:YA:2147:G:C8    | 2.47                     | 0.50              |
| 26:YB:74:U:H2'     | 26:YB:75:G:O4'     | 2.10                     | 0.50              |
| 27:YD:10:THR:HG23  | 27:YD:13:ARG:CB    | 2.34                     | 0.50              |
| 29:YF:32:LEU:O     | 29:YF:36:VAL:HG23  | 2.11                     | 0.50              |
| 33:YN:78:TYR:N     | 33:YN:78:TYR:HD1   | 2.07                     | 0.50              |
| 33:YN:112:LEU:HD23 | 33:YN:113:GLY:N    | 2.26                     | 0.50              |
| 34:YO:23:ARG:HH11  | 34:YO:23:ARG:HG2   | 1.76                     | 0.50              |
| 34:YO:113:LYS:O    | 34:YO:116:SER:HB3  | 2.11                     | 0.50              |
| 37:YR:3:HIS:C      | 37:YR:5:LYS:H      | 2.17                     | 0.50              |
| 40:YU:112:ARG:HG2  | 40:YU:112:ARG:HH11 | 1.76                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:QB:200:ILE:O    | 2:QB:201:ILE:HD13  | 2.11                     | 0.50              |
| 6:QF:63:TYR:N     | 6:QF:63:TYR:CD2    | 2.79                     | 0.50              |
| 8:QH:51:VAL:HG11  | 8:QH:60:ARG:HG3    | 1.92                     | 0.50              |
| 8:QH:83:ILE:HB    | 8:QH:137:VAL:HG13  | 1.93                     | 0.50              |
| 9:QI:10:ARG:HG3   | 9:QI:105:ASP:HB2   | 1.92                     | 0.50              |
| 14:QN:43:CYS:O    | 14:QN:46:GLU:N     | 2.43                     | 0.50              |
| 16:QP:83:GLU:HG3  | 16:QP:84:ALA:H     | 1.77                     | 0.50              |
| 18:QR:43:PHE:C    | 18:QR:44:LEU:HD12  | 2.36                     | 0.50              |
| 20:QT:98:PRO:C    | 20:QT:100:ILE:H    | 2.18                     | 0.50              |
| 22:QV:68:C:H2'    | 22:QV:69:C:H6      | 1.76                     | 0.50              |
| 25:RA:74:A:H4'    | 25:RA:75:G:O5'     | 2.11                     | 0.50              |
| 25:RA:1427:A:H4'  | 25:RA:1428:C:O5'   | 2.11                     | 0.50              |
| 25:RA:2116:G:H1   | 25:RA:2162:G:P     | 2.34                     | 0.50              |
| 25:RA:2466:C:H5'  | 55:R9:5:ALA:HB3    | 1.93                     | 0.50              |
| 30:RG:92:VAL:O    | 30:RG:92:VAL:HG13  | 2.12                     | 0.50              |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA2  | 1.91                     | 0.50              |
| 35:RP:101:VAL:HA  | 35:RP:105:LEU:O    | 2.10                     | 0.50              |
| 36:RQ:133:ARG:HG2 | 36:RQ:134:ARG:N    | 2.26                     | 0.50              |
| 38:RS:35:ILE:CD1  | 38:RS:101:LEU:HD23 | 2.41                     | 0.50              |
| 39:RT:54:ARG:HG2  | 39:RT:54:ARG:NH1   | 2.23                     | 0.50              |
| 44:RY:2:ARG:HG2   | 44:RY:2:ARG:NH1    | 2.22                     | 0.50              |
| 44:RY:74:PRO:O    | 44:RY:80:GLY:HA2   | 2.10                     | 0.50              |
| 51:R5:36:CYS:C    | 51:R5:38:ALA:H     | 2.19                     | 0.50              |
| 1:XA:458:C:H2'    | 1:XA:464:G:H8      | 1.76                     | 0.50              |
| 1:XA:923:A:O2'    | 1:XA:1399:C:OP2    | 2.24                     | 0.50              |
| 1:XA:1128:C:H5'   | 9:XI:16:ARG:NH2    | 2.27                     | 0.50              |
| 1:XA:1226:C:O2'   | 13:XM:111:LYS:NZ   | 2.42                     | 0.50              |
| 1:XA:1372:U:H2'   | 1:XA:1373:G:O4'    | 2.11                     | 0.50              |
| 4:XD:108:LEU:HD11 | 4:XD:174:LEU:CD2   | 2.37                     | 0.50              |
| 9:XI:48:GLU:N     | 9:XI:49:PRO:CD     | 2.74                     | 0.50              |
| 9:XI:53:VAL:HG21  | 9:XI:92:TYR:CZ     | 2.45                     | 0.50              |
| 9:XI:79:LEU:HD22  | 9:XI:101:PHE:O     | 2.10                     | 0.50              |
| 25:YA:2749:A:H4'  | 31:YH:62:LYS:HB3   | 1.93                     | 0.50              |
| 29:YF:108:LYS:HA  | 29:YF:108:LYS:NZ   | 2.27                     | 0.50              |
| 37:YR:92:GLY:N    | 37:YR:94:TYR:HE2   | 2.10                     | 0.50              |
| 39:YT:57:PHE:CG   | 39:YT:58:ASN:N     | 2.79                     | 0.50              |
| 44:YY:75:ILE:CG1  | 44:YY:76:CYS:N     | 2.73                     | 0.50              |
| 45:YZ:141:VAL:CG2 | 45:YZ:144:LEU:HB2  | 2.41                     | 0.50              |
| 47:Y1:94:LEU:O    | 47:Y1:95:LEU:HG    | 2.11                     | 0.50              |
| 50:Y4:1:MET:HE3   | 50:Y4:6:HIS:CD2    | 2.46                     | 0.50              |
| 53:Y7:36:GLN:HG2  | 53:Y7:36:GLN:O     | 2.09                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:1095:U:OP1    | 1:QA:1108:G:N1    | 2.40                     | 0.50              |
| 2:QB:53:ARG:HA     | 2:QB:56:ARG:HG3   | 1.93                     | 0.50              |
| 3:QC:34:LEU:O      | 3:QC:38:ARG:HG3   | 2.11                     | 0.50              |
| 8:QH:95:VAL:HB     | 8:QH:99:GLU:O     | 2.12                     | 0.50              |
| 13:QM:66:LEU:O     | 13:QM:70:LEU:HB2  | 2.11                     | 0.50              |
| 16:QP:59:TRP:HA    | 16:QP:59:TRP:HE3  | 1.77                     | 0.50              |
| 25:RA:2150:U:H2'   | 25:RA:2151:G:H8   | 1.75                     | 0.50              |
| 25:RA:2283:C:P     | 52:R6:5:VAL:HG13  | 2.52                     | 0.50              |
| 25:RA:2646:C:H2'   | 25:RA:2647:U:O4'  | 2.12                     | 0.50              |
| 28:RE:37:ARG:HE    | 28:RE:37:ARG:H    | 1.59                     | 0.50              |
| 29:RF:45:ARG:CG    | 29:RF:45:ARG:NH1  | 2.71                     | 0.50              |
| 29:RF:108:LYS:HA   | 29:RF:108:LYS:NZ  | 2.27                     | 0.50              |
| 31:RH:169:VAL:HG13 | 31:RH:170:ARG:N   | 2.26                     | 0.50              |
| 34:RO:24:VAL:O     | 34:RO:24:VAL:HG13 | 2.11                     | 0.50              |
| 38:RS:62:LYS:HB3   | 38:RS:97:ARG:CD   | 2.39                     | 0.50              |
| 40:RU:98:LEU:HD23  | 40:RU:98:LEU:C    | 2.35                     | 0.50              |
| 1:XA:397:A:H5'     | 1:XA:398:C:OP1    | 2.12                     | 0.50              |
| 1:XA:686:U:O4      | 1:XA:703:G:O2'    | 2.30                     | 0.50              |
| 2:XB:24:TRP:CE3    | 2:XB:26:PRO:HA    | 2.45                     | 0.50              |
| 9:XI:10:ARG:HG3    | 9:XI:105:ASP:HB2  | 1.92                     | 0.50              |
| 9:XI:83:ARG:HA     | 9:XI:86:VAL:CG1   | 2.42                     | 0.50              |
| 15:XO:17:ARG:NH1   | 15:XO:77:ARG:NH1  | 2.59                     | 0.50              |
| 23:XY:40:G:H2'     | 23:XY:41:A:H5'    | 1.94                     | 0.50              |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:H8 | 1.76                     | 0.50              |
| 25:YA:898:C:C2'    | 25:YA:899:A:H5'   | 2.42                     | 0.50              |
| 25:YA:1332:G:H21   | 25:YA:1610:A:H8   | 1.58                     | 0.50              |
| 26:YB:49:C:H2'     | 26:YB:50:G:H8     | 1.75                     | 0.50              |
| 30:YG:6:ALA:H      | 50:Y4:23:GLU:CG   | 2.25                     | 0.50              |
| 31:YH:131:VAL:CG1  | 31:YH:132:ARG:N   | 2.74                     | 0.50              |
| 31:YH:169:VAL:HG13 | 31:YH:170:ARG:N   | 2.26                     | 0.50              |
| 36:YQ:132:VAL:HG12 | 36:YQ:133:ARG:N   | 2.27                     | 0.50              |
| 38:YS:26:LEU:HD22  | 38:YS:87:PHE:CD1  | 2.46                     | 0.50              |
| 41:YV:51:VAL:CG1   | 41:YV:52:VAL:H    | 2.22                     | 0.50              |
| 42:YW:22:ASP:HA    | 42:YW:25:ARG:HH12 | 1.75                     | 0.50              |
| 47:Y1:87:PRO:O     | 47:Y1:91:LYS:HB2  | 2.10                     | 0.50              |
| 48:Y2:41:ILE:HD11  | 48:Y2:44:LEU:CB   | 2.42                     | 0.50              |
| 49:Y3:17:LYS:HA    | 49:Y3:20:LYS:HD2  | 1.92                     | 0.50              |
| 1:QA:297:G:N2      | 1:QA:300:A:OP2    | 2.45                     | 0.50              |
| 1:QA:452:A:O2'     | 1:QA:453:A:O4'    | 2.26                     | 0.50              |
| 1:QA:978:A:N7      | 1:QA:1361:G:N2    | 2.59                     | 0.50              |
| 1:QA:1095:U:P      | 1:QA:1108:G:H1    | 2.34                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1305:G:HO2'   | 1:QA:1306:A:H8     | 1.59                     | 0.50              |
| 3:QC:34:LEU:HD23   | 3:QC:34:LEU:C      | 2.37                     | 0.50              |
| 3:QC:139:GLN:O     | 3:QC:143:GLU:HB2   | 2.11                     | 0.50              |
| 4:QD:162:LEU:HD13  | 4:QD:181:MET:HB3   | 1.93                     | 0.50              |
| 25:RA:1470:G:N2    | 25:RA:1522:G:OP2   | 2.44                     | 0.50              |
| 25:RA:1694:C:O2'   | 25:RA:1695:G:OP2   | 2.25                     | 0.50              |
| 25:RA:2031:A:N3    | 25:RA:2455:G:O2'   | 2.41                     | 0.50              |
| 28:RE:61:ARG:CB    | 28:RE:62:PRO:HD3   | 2.41                     | 0.50              |
| 28:RE:176:ILE:HG22 | 28:RE:176:ILE:O    | 2.10                     | 0.50              |
| 28:RE:203:LYS:HE3  | 28:RE:204:ALA:CB   | 2.40                     | 0.50              |
| 30:RG:43:LEU:O     | 30:RG:88:ILE:HG12  | 2.12                     | 0.50              |
| 30:RG:121:ASN:C    | 30:RG:123:ASN:H    | 2.20                     | 0.50              |
| 33:RN:129:PRO:C    | 33:RN:131:GLN:H    | 2.20                     | 0.50              |
| 37:RR:70:LEU:O     | 37:RR:72:ASP:N     | 2.42                     | 0.50              |
| 39:RT:51:ARG:HG3   | 39:RT:98:LYS:HG3   | 1.93                     | 0.50              |
| 40:RU:92:ARG:C     | 40:RU:94:ASN:N     | 2.69                     | 0.50              |
| 43:RX:35:THR:O     | 43:RX:36:LYS:C     | 2.55                     | 0.50              |
| 45:RZ:110:GLY:N    | 45:RZ:111:VAL:HG12 | 2.27                     | 0.50              |
| 51:R5:48:GLU:HA    | 51:R5:59:GLU:HG2   | 1.94                     | 0.50              |
| 1:XA:131:C:H2'     | 1:XA:132:C:C6      | 2.45                     | 0.50              |
| 1:XA:250:A:H4'     | 1:XA:251:G:O5'     | 2.10                     | 0.50              |
| 1:XA:537:G:H5''    | 12:XL:113:ARG:HH12 | 1.76                     | 0.50              |
| 1:XA:1199:U:H4'    | 10:XJ:54:PHE:CE2   | 2.47                     | 0.50              |
| 1:XA:1220:G:O3'    | 19:XS:36:ARG:HD3   | 2.12                     | 0.50              |
| 1:XA:1322:C:H5'    | 13:XM:100:GLY:HA2  | 1.93                     | 0.50              |
| 8:XH:102:ARG:NH1   | 8:XH:105:ARG:HH12  | 2.09                     | 0.50              |
| 11:XK:106:LYS:O    | 11:XK:107:SER:HB3  | 2.12                     | 0.50              |
| 14:XN:48:ALA:CA    | 14:XN:53:LEU:HD12  | 2.42                     | 0.50              |
| 16:XP:83:GLU:HG3   | 16:XP:84:ALA:H     | 1.77                     | 0.50              |
| 19:XS:50:ALA:CB    | 19:XS:57:HIS:HB3   | 2.37                     | 0.50              |
| 25:YA:2477:C:H2'   | 55:Y9:1:MET:HG3    | 1.94                     | 0.50              |
| 25:YA:2500:U:O2'   | 25:YA:2504:U:OP1   | 2.27                     | 0.50              |
| 25:YA:2808:U:H5'   | 25:YA:2891:G:O6    | 2.11                     | 0.50              |
| 30:YG:43:LEU:O     | 30:YG:88:ILE:HG12  | 2.12                     | 0.50              |
| 30:YG:111:LEU:N    | 30:YG:112:PRO:CD   | 2.75                     | 0.50              |
| 31:YH:16:SER:O     | 31:YH:17:VAL:HG23  | 2.12                     | 0.50              |
| 31:YH:133:VAL:HG12 | 31:YH:141:VAL:HG13 | 1.93                     | 0.50              |
| 33:YN:120:LEU:C    | 33:YN:120:LEU:HD13 | 2.37                     | 0.50              |
| 34:YO:15:GLY:O     | 34:YO:46:ALA:HB1   | 2.10                     | 0.50              |
| 37:YR:85:PRO:C     | 37:YR:87:TYR:H     | 2.18                     | 0.50              |
| 38:YS:89:ARG:HD2   | 38:YS:89:ARG:O     | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:YV:29:PRO:O     | 41:YV:61:VAL:O     | 2.29                     | 0.50              |
| 50:Y4:57:GLU:O     | 50:Y4:61:ARG:O     | 2.30                     | 0.50              |
| 56:Z8:76:PPU:HD2   | 56:Z8:76:PPU:HN2   | 1.76                     | 0.50              |
| 1:QA:401:C:O2'     | 1:QA:621:A:N3      | 2.42                     | 0.50              |
| 1:QA:1077:G:N2     | 1:QA:1080:A:OP2    | 2.38                     | 0.50              |
| 2:QB:170:GLU:HA    | 2:QB:172:ILE:CD1   | 2.41                     | 0.50              |
| 3:QC:184:TYR:HA    | 3:QC:200:ALA:O     | 2.12                     | 0.50              |
| 7:QG:50:ILE:HG21   | 7:QG:58:PRO:HA     | 1.93                     | 0.50              |
| 9:QI:5:TYR:HA      | 9:QI:17:VAL:O      | 2.12                     | 0.50              |
| 9:QI:48:GLU:N      | 9:QI:49:PRO:CD     | 2.74                     | 0.50              |
| 9:QI:53:VAL:HG21   | 9:QI:92:TYR:CZ     | 2.46                     | 0.50              |
| 10:QJ:56:HIS:O     | 10:QJ:58:ASP:O     | 2.30                     | 0.50              |
| 10:QJ:98:ILE:H     | 10:QJ:98:ILE:CD1   | 2.25                     | 0.50              |
| 11:QK:91:ARG:NH2   | 18:QR:88:LYS:HZ1   | 2.09                     | 0.50              |
| 14:QN:48:ALA:CA    | 14:QN:53:LEU:HD12  | 2.42                     | 0.50              |
| 15:QO:26:GLU:OE2   | 15:QO:77:ARG:NH1   | 2.43                     | 0.50              |
| 25:RA:372:G:H5''   | 47:R1:66:HIS:CD2   | 2.47                     | 0.50              |
| 25:RA:2377:A:H4'   | 38:RS:111:GLU:O    | 2.12                     | 0.50              |
| 27:RD:35:LYS:HD2   | 27:RD:104:TYR:CD1  | 2.45                     | 0.50              |
| 27:RD:237:GLU:OE1  | 27:RD:237:GLU:HA   | 2.12                     | 0.50              |
| 28:RE:119:ARG:HD3  | 28:RE:160:TYR:CD2  | 2.46                     | 0.50              |
| 30:RG:109:VAL:O    | 30:RG:113:ARG:HG3  | 2.10                     | 0.50              |
| 33:RN:46:VAL:O     | 33:RN:47:ALA:CB    | 2.57                     | 0.50              |
| 33:RN:137:LYS:HG3  | 33:RN:138:LEU:H    | 1.77                     | 0.50              |
| 35:RP:114:ILE:HD13 | 35:RP:125:VAL:CG2  | 2.41                     | 0.50              |
| 36:RQ:2:LEU:HD23   | 36:RQ:2:LEU:N      | 2.27                     | 0.50              |
| 36:RQ:108:GLY:O    | 36:RQ:109:VAL:HG23 | 2.12                     | 0.50              |
| 38:RS:26:LEU:CD2   | 38:RS:87:PHE:CD1   | 2.95                     | 0.50              |
| 40:RU:92:ARG:NH1   | 40:RU:95:LEU:HD11  | 2.26                     | 0.50              |
| 42:RW:34:ASN:O     | 42:RW:35:ILE:C     | 2.55                     | 0.50              |
| 42:RW:40:ASN:C     | 42:RW:41:LYS:HG2   | 2.36                     | 0.50              |
| 44:RY:48:ALA:HB2   | 44:RY:61:ILE:CD1   | 2.41                     | 0.50              |
| 44:RY:88:LYS:NZ    | 44:RY:88:LYS:HA    | 2.27                     | 0.50              |
| 50:R4:1:MET:O      | 50:R4:1:MET:HG3    | 2.12                     | 0.50              |
| 50:R4:1:MET:HE3    | 50:R4:6:HIS:CD2    | 2.46                     | 0.50              |
| 51:R5:54:GLY:O     | 51:R5:55:ARG:C     | 2.54                     | 0.50              |
| 1:XA:667:G:H4'     | 15:XO:51:HIS:CE1   | 2.46                     | 0.50              |
| 1:XA:1221:G:O3'    | 19:XS:77:THR:HG21  | 2.11                     | 0.50              |
| 2:XB:23:ARG:HG2    | 2:XB:23:ARG:HH11   | 1.76                     | 0.50              |
| 3:XC:11:ARG:HG3    | 3:XC:15:THR:HG21   | 1.93                     | 0.50              |
| 3:XC:34:LEU:O      | 3:XC:38:ARG:HG3    | 2.10                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:YN:41:ARG:HE   | 14:YN:42:ILE:HG13  | 1.76                     | 0.50              |
| 15:XO:17:ARG:NH1  | 15:XO:77:ARG:CZ    | 2.74                     | 0.50              |
| 19:XS:26:GLY:O    | 19:XS:27:GLU:HB2   | 2.11                     | 0.50              |
| 25:YA:774:A:H2    | 25:YA:787:U:O2'    | 1.93                     | 0.50              |
| 25:YA:2275:C:O2   | 36:YQ:83:MET:HG3   | 2.11                     | 0.50              |
| 25:YA:2712:U:O2'  | 25:YA:2712(A):A:P  | 2.70                     | 0.50              |
| 27:YD:233:HIS:CD2 | 27:YD:233:HIS:H    | 2.29                     | 0.50              |
| 27:YD:241:PRO:O   | 27:YD:242:ARG:C    | 2.53                     | 0.50              |
| 28:YE:2:LYS:HG2   | 28:YE:95:ILE:CG2   | 2.42                     | 0.50              |
| 30:YG:16:ARG:HB3  | 30:YG:17:PRO:HD3   | 1.94                     | 0.50              |
| 31:YH:24:VAL:HG21 | 31:YH:72:ILE:HG12  | 1.93                     | 0.50              |
| 34:YO:35:VAL:O    | 34:YO:35:VAL:HG23  | 2.11                     | 0.50              |
| 35:YP:64:LYS:C    | 35:YP:66:GLY:N     | 2.56                     | 0.50              |
| 35:YP:147:LEU:O   | 35:YP:148:LEU:HB2  | 2.11                     | 0.50              |
| 36:YQ:36:ALA:HB1  | 36:YQ:127:ILE:HD12 | 1.93                     | 0.50              |
| 40:YU:92:ARG:C    | 40:YU:94:ASN:N     | 2.70                     | 0.50              |
| 42:YW:40:ASN:C    | 42:YW:41:LYS:HG2   | 2.36                     | 0.50              |
| 42:YW:70:TYR:N    | 42:YW:70:TYR:CD2   | 2.75                     | 0.50              |
| 44:YY:2:ARG:O     | 44:YY:3:VAL:C      | 2.55                     | 0.50              |
| 44:YY:46:LYS:HE3  | 44:YY:63:LYS:HB3   | 1.93                     | 0.50              |
| 44:YY:48:ALA:HB2  | 44:YY:61:ILE:CD1   | 2.41                     | 0.50              |
| 52:Y6:9:LEU:HB3   | 52:Y6:26:ASN:O     | 2.11                     | 0.50              |
| 53:Y7:9:ARG:HH12  | 53:Y7:47:ARG:HG3   | 1.76                     | 0.50              |
| 53:Y7:12:ARG:NH1  | 53:Y7:12:ARG:HG3   | 2.27                     | 0.50              |
| 1:QA:191(F):U:O2  | 20:QT:105:SER:HB2  | 2.11                     | 0.50              |
| 1:QA:1118:C:OP1   | 9:QI:9:ARG:HD3     | 2.12                     | 0.50              |
| 1:QA:1305:G:OP1   | 21:QU:2:GLY:HA2    | 2.12                     | 0.50              |
| 3:QC:8:ILE:C      | 3:QC:10:PHE:N      | 2.69                     | 0.50              |
| 3:QC:70:VAL:CG1   | 3:QC:71:ALA:N      | 2.73                     | 0.50              |
| 4:QD:178:VAL:O    | 4:QD:180:GLY:N     | 2.44                     | 0.50              |
| 8:QH:20:TYR:HD1   | 8:QH:65:TYR:HD2    | 1.55                     | 0.50              |
| 10:QJ:22:LYS:NZ   | 10:QJ:23:ILE:HG12  | 2.27                     | 0.50              |
| 13:QM:28:ALA:C    | 13:QM:30:ALA:N     | 2.70                     | 0.50              |
| 14:QN:22:THR:O    | 14:QN:23:ARG:CB    | 2.59                     | 0.50              |
| 25:RA:827:U:H1'   | 25:RA:2246:G:O2'   | 2.12                     | 0.50              |
| 25:RA:2010:G:H5'' | 42:RW:42:ARG:HB2   | 1.93                     | 0.50              |
| 25:RA:2469:A:H5'  | 25:RA:2470:G:OP2   | 2.12                     | 0.50              |
| 27:RD:2:ALA:CB    | 27:RD:20:ASP:CB    | 2.90                     | 0.50              |
| 27:RD:28:GLU:OE1  | 27:RD:29:PRO:HD2   | 2.11                     | 0.50              |
| 27:RD:31:LYS:C    | 27:RD:32:SER:O     | 2.54                     | 0.50              |
| 27:RD:32:SER:O    | 27:RD:33:LEU:CB    | 2.60                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:2:LYS:HG2    | 28:RE:95:ILE:CG2   | 2.42                     | 0.50              |
| 31:RH:16:SER:O     | 31:RH:17:VAL:HG23  | 2.12                     | 0.50              |
| 31:RH:133:VAL:HG12 | 31:RH:141:VAL:HG13 | 1.93                     | 0.50              |
| 33:RN:120:LEU:HD13 | 33:RN:120:LEU:C    | 2.37                     | 0.50              |
| 37:RR:96:ARG:NH2   | 37:RR:117:VAL:HG23 | 2.27                     | 0.50              |
| 38:RS:74:ALA:O     | 38:RS:75:GLU:C     | 2.54                     | 0.50              |
| 39:RT:23:ARG:CB    | 39:RT:24:PRO:HD2   | 2.40                     | 0.50              |
| 42:RW:22:ASP:HA    | 42:RW:25:ARG:HH12  | 1.75                     | 0.50              |
| 44:RY:16:ALA:O     | 44:RY:21:LYS:HD3   | 2.11                     | 0.50              |
| 51:R5:50:GLY:O     | 51:R5:51:TYR:CB    | 2.59                     | 0.50              |
| 52:R6:9:LEU:HD13   | 52:R6:26:ASN:HD22  | 1.77                     | 0.50              |
| 52:R6:34:LEU:HD23  | 52:R6:36:LEU:HD22  | 1.92                     | 0.50              |
| 52:R6:41:PRO:HD2   | 52:R6:46:HIS:H     | 1.77                     | 0.50              |
| 55:R9:7:VAL:HG12   | 55:R9:25:VAL:HG21  | 1.94                     | 0.50              |
| 1:XA:60:A:P        | 1:XA:60:A:H8       | 2.35                     | 0.50              |
| 3:XC:34:LEU:HD23   | 3:XC:34:LEU:C      | 2.37                     | 0.50              |
| 4:XD:54:TYR:CE1    | 4:XD:206:PHE:HE1   | 2.29                     | 0.50              |
| 7:XG:50:ILE:HA     | 7:XG:54:THR:HG22   | 1.94                     | 0.50              |
| 7:XG:150:ALA:HA    | 11:XK:59:TYR:CD2   | 2.47                     | 0.50              |
| 10:XJ:40:LEU:HB2   | 10:XJ:69:ASN:CB    | 2.40                     | 0.50              |
| 21:XU:6:ARG:HH21   | 21:XU:15:ARG:NE    | 2.09                     | 0.50              |
| 25:YA:587:C:H4'    | 25:YA:588:U:O5'    | 2.12                     | 0.50              |
| 25:YA:1853:A:N3    | 25:YA:2233:U:O2'   | 2.38                     | 0.50              |
| 26:YB:52:A:H62     | 38:YS:33:LYS:HG3   | 1.76                     | 0.50              |
| 27:YD:182:LEU:H    | 27:YD:272:ALA:CB   | 2.25                     | 0.50              |
| 28:YE:105:THR:HB   | 28:YE:197:ILE:HG12 | 1.93                     | 0.50              |
| 30:YG:103:LEU:HD21 | 30:YG:178:PHE:CZ   | 2.47                     | 0.50              |
| 34:YO:105:GLU:O    | 34:YO:108:GLU:HB2  | 2.12                     | 0.50              |
| 35:YP:138:LEU:HD11 | 35:YP:144:GLU:CG   | 2.42                     | 0.50              |
| 36:YQ:108:GLY:O    | 36:YQ:109:VAL:HG23 | 2.12                     | 0.50              |
| 37:YR:28:LEU:CD2   | 37:YR:114:VAL:HG12 | 2.41                     | 0.50              |
| 40:YU:92:ARG:CD    | 40:YU:94:ASN:HB3   | 2.42                     | 0.50              |
| 41:YV:51:VAL:CG1   | 41:YV:52:VAL:N     | 2.75                     | 0.50              |
| 44:YY:19:LYS:O     | 44:YY:19:LYS:CG    | 2.59                     | 0.50              |
| 44:YY:101:LYS:O    | 44:YY:102:CYS:SG   | 2.67                     | 0.50              |
| 45:YZ:53:ILE:HG22  | 45:YZ:71:VAL:HG22  | 1.92                     | 0.50              |
| 46:Y0:27:GLU:HB2   | 46:Y0:69:PHE:HD1   | 1.77                     | 0.50              |
| 49:Y3:7:LYS:CB     | 49:Y3:34:GLU:HG2   | 2.41                     | 0.50              |
| 1:QA:191(D):U:H2'  | 1:QA:191(E):G:C8   | 2.46                     | 0.50              |
| 1:QA:713:G:H2'     | 1:QA:714:G:C8      | 2.46                     | 0.50              |
| 1:QA:738:C:H5''    | 6:QF:69:GLU:HB2    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:15:VAL:H      | 2:QB:16:HIS:HD1    | 1.59                     | 0.50              |
| 3:QC:11:ARG:HG3    | 3:QC:15:THR:HG21   | 1.94                     | 0.50              |
| 3:QC:52:LEU:H      | 3:QC:52:LEU:CD2    | 2.20                     | 0.50              |
| 3:QC:87:LEU:C      | 3:QC:89:GLU:H      | 2.19                     | 0.50              |
| 4:QD:128:VAL:O     | 4:QD:130:GLY:N     | 2.45                     | 0.50              |
| 8:QH:84:ARG:O      | 8:QH:135:CYS:HB2   | 2.12                     | 0.50              |
| 14:QN:23:ARG:C     | 14:QN:24:CYS:O     | 2.54                     | 0.50              |
| 16:QP:13:HIS:C     | 16:QP:15:PRO:HD3   | 2.36                     | 0.50              |
| 19:QS:41:VAL:CG1   | 19:QS:45:VAL:N     | 2.74                     | 0.50              |
| 20:QT:49:ALA:CB    | 20:QT:99:LEU:HD22  | 2.42                     | 0.50              |
| 21:QU:2:GLY:O      | 21:QU:4:GLY:N      | 2.45                     | 0.50              |
| 25:RA:384:U:H2'    | 25:RA:385:C:H6     | 1.77                     | 0.50              |
| 25:RA:863:A:H2'    | 25:RA:864:G:C8     | 2.47                     | 0.50              |
| 25:RA:1105:U:H2'   | 25:RA:1106:G:H8    | 1.77                     | 0.50              |
| 25:RA:1578:U:H2'   | 25:RA:1579:A:H5'   | 1.93                     | 0.50              |
| 25:RA:2154:G:H2'   | 25:RA:2155:G:C8    | 2.47                     | 0.50              |
| 30:RG:111:LEU:N    | 30:RG:112:PRO:CD   | 2.75                     | 0.50              |
| 31:RH:103:LEU:CD1  | 31:RH:131:VAL:HG21 | 2.41                     | 0.50              |
| 35:RP:6:LEU:N      | 35:RP:6:LEU:CD2    | 2.75                     | 0.50              |
| 35:RP:61:ARG:HH21  | 54:R8:13:ARG:HD2   | 1.77                     | 0.50              |
| 37:RR:92:GLY:N     | 37:RR:94:TYR:HE2   | 2.10                     | 0.50              |
| 38:RS:60:GLY:O     | 38:RS:61:ASN:CB    | 2.55                     | 0.50              |
| 39:RT:38:ASN:O     | 39:RT:39:ARG:O     | 2.30                     | 0.50              |
| 47:R1:80:LEU:HB2   | 47:R1:81:LYS:CE    | 2.41                     | 0.50              |
| 48:R2:16:LEU:O     | 48:R2:17:SER:CB    | 2.56                     | 0.50              |
| 56:Z6:76:PPU:HN2   | 56:Z6:76:PPU:HD2   | 1.76                     | 0.50              |
| 1:XA:1431:C:H2'    | 1:XA:1432:G:O4'    | 2.12                     | 0.50              |
| 1:XA:1499:A:H1'    | 1:XA:1520:G:H5'    | 1.93                     | 0.50              |
| 2:XB:200:ILE:O     | 2:XB:201:ILE:HD13  | 2.12                     | 0.50              |
| 4:XD:20:TYR:CD2    | 4:XD:27:TYR:CD2    | 3.00                     | 0.50              |
| 8:XH:95:VAL:HB     | 8:XH:99:GLU:O      | 2.12                     | 0.50              |
| 11:XK:25:TYR:CD1   | 11:XK:25:TYR:N     | 2.80                     | 0.50              |
| 13:XM:102:ARG:O    | 13:XM:102:ARG:HG3  | 2.11                     | 0.50              |
| 20:XT:49:ALA:CB    | 20:XT:99:LEU:HD22  | 2.42                     | 0.50              |
| 25:YA:103:A:H8     | 25:YA:103:A:O5'    | 1.94                     | 0.50              |
| 25:YA:185:U:H4'    | 25:YA:218:A:H4'    | 1.94                     | 0.50              |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:H8  | 1.76                     | 0.50              |
| 25:YA:357:A:H2'    | 25:YA:358:U:C6     | 2.47                     | 0.50              |
| 25:YA:507:A:H5''   | 25:YA:508:G:H5'    | 1.93                     | 0.50              |
| 25:YA:807:U:O2'    | 25:YA:2060:A:N1    | 2.41                     | 0.50              |
| 25:YA:1341:U:P     | 25:YA:1397:U:H3    | 2.34                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2208:U:H1'  | 27:YD:151:LYS:HE2  | 1.94                     | 0.50              |
| 25:YA:2287:A:N6   | 25:YA:2344:U:H3    | 2.08                     | 0.50              |
| 27:YD:35:LYS:HE2  | 27:YD:104:TYR:HB2  | 1.94                     | 0.50              |
| 36:YQ:23:GLY:O    | 36:YQ:24:GLY:C     | 2.54                     | 0.50              |
| 37:YR:10:LEU:O    | 37:YR:11:ASN:C     | 2.55                     | 0.50              |
| 38:YS:35:ILE:CD1  | 38:YS:101:LEU:HD23 | 2.41                     | 0.50              |
| 43:YX:47:PHE:O    | 43:YX:48:LYS:C     | 2.55                     | 0.50              |
| 50:Y4:22:ILE:H    | 50:Y4:22:ILE:HD12  | 1.77                     | 0.50              |
| 50:Y4:42:PHE:CD1  | 50:Y4:42:PHE:C     | 2.90                     | 0.50              |
| 2:QB:16:HIS:HB3   | 2:QB:210:SER:CB    | 2.42                     | 0.50              |
| 4:QD:13:ARG:HH22  | 4:QD:36:ARG:CZ     | 2.24                     | 0.50              |
| 4:QD:28:SER:CB    | 4:QD:29:PRO:CD     | 2.85                     | 0.50              |
| 7:QG:108:ALA:C    | 7:QG:110:GLN:H     | 2.19                     | 0.50              |
| 16:QP:39:TYR:OH   | 16:QP:41:PRO:HB3   | 2.11                     | 0.50              |
| 25:RA:288:C:H2'   | 25:RA:289:A:H8     | 1.77                     | 0.50              |
| 25:RA:1790:C:H5'' | 25:RA:1791:A:OP1   | 2.12                     | 0.50              |
| 25:RA:2695:C:H2'  | 25:RA:2696:U:C6    | 2.47                     | 0.50              |
| 25:RA:2712:U:OP1  | 25:RA:2714:G:H4'   | 2.12                     | 0.50              |
| 27:RD:35:LYS:HE2  | 27:RD:104:TYR:HB2  | 1.94                     | 0.50              |
| 27:RD:218:ARG:HB3 | 27:RD:219:PRO:HD2  | 1.94                     | 0.50              |
| 29:RF:11:VAL:CG1  | 29:RF:12:LEU:N     | 2.75                     | 0.50              |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:HG23  | 1.93                     | 0.50              |
| 34:RO:104:ARG:NE  | 39:RT:34:VAL:HG11  | 2.26                     | 0.50              |
| 35:RP:81:GLN:CD   | 35:RP:106:LEU:O    | 2.55                     | 0.50              |
| 36:RQ:80:GLU:HG3  | 36:RQ:81:VAL:N     | 2.27                     | 0.50              |
| 38:RS:83:LYS:HG2  | 38:RS:109:GLY:HA2  | 1.90                     | 0.50              |
| 40:RU:76:TYR:CD2  | 40:RU:76:TYR:C     | 2.90                     | 0.50              |
| 44:RY:90:LEU:HD22 | 44:RY:90:LEU:H     | 1.73                     | 0.50              |
| 47:R1:82:LEU:HD13 | 47:R1:83:GLU:C     | 2.35                     | 0.50              |
| 1:XA:310:G:H4'    | 16:XP:31:LYS:HD3   | 1.93                     | 0.50              |
| 1:XA:1226:C:O2'   | 13:XM:103:THR:O    | 2.15                     | 0.50              |
| 2:XB:16:HIS:HB3   | 2:XB:210:SER:CB    | 2.42                     | 0.50              |
| 3:XC:132:ARG:O    | 3:XC:136:GLN:HB2   | 2.11                     | 0.50              |
| 4:XD:150:GLU:C    | 4:XD:152:SER:H     | 2.20                     | 0.50              |
| 10:XJ:54:PHE:O    | 10:XJ:55:LYS:HG3   | 2.11                     | 0.50              |
| 12:XL:8:ASN:OD1   | 17:XQ:34:LYS:HE2   | 2.12                     | 0.50              |
| 13:XM:14:ARG:HG3  | 13:XM:16:ASP:OD2   | 2.12                     | 0.50              |
| 20:XT:84:LEU:HD13 | 20:XT:84:LEU:C     | 2.37                     | 0.50              |
| 25:YA:222:A:O2'   | 25:YA:223:A:O5'    | 2.30                     | 0.50              |
| 25:YA:654:A:O2'   | 25:YA:654(A):G:N7  | 2.40                     | 0.50              |
| 25:YA:2022:U:O2'  | 25:YA:2617:C:H5'   | 2.12                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:YB:44:G:O2'     | 26:YB:47:C:N4     | 2.44                     | 0.50              |
| 27:YD:218:ARG:HB3  | 27:YD:219:PRO:HD2 | 1.94                     | 0.50              |
| 29:YF:53:THR:C     | 29:YF:55:GLY:N    | 2.68                     | 0.50              |
| 31:YH:7:LEU:C      | 31:YH:7:LEU:HD12  | 2.37                     | 0.50              |
| 32:YI:144:VAL:HG22 | 32:YI:145:VAL:H   | 1.77                     | 0.50              |
| 34:YO:104:ARG:NE   | 39:YT:34:VAL:HG11 | 2.26                     | 0.50              |
| 35:YP:88:LEU:C     | 35:YP:88:LEU:HD23 | 2.36                     | 0.50              |
| 38:YS:5:THR:HG1    | 38:YS:7:TYR:HB3   | 1.75                     | 0.50              |
| 40:YU:76:TYR:CD2   | 40:YU:76:TYR:C    | 2.90                     | 0.50              |
| 42:YW:1:MET:HE2    | 42:YW:2:GLU:H     | 1.77                     | 0.50              |
| 47:Y1:81:LYS:O     | 47:Y1:82:LEU:O    | 2.30                     | 0.50              |
| 48:Y2:9:GLN:O      | 48:Y2:12:GLU:HB3  | 2.10                     | 0.50              |
| 51:Y5:37:LYS:O     | 51:Y5:37:LYS:HD2  | 2.12                     | 0.50              |
| 51:Y5:50:GLY:O     | 51:Y5:51:TYR:CB   | 2.59                     | 0.50              |
| 1:QA:1326:C:OP1    | 21:QU:17:THR:OG1  | 2.27                     | 0.49              |
| 3:QC:35:GLU:O      | 3:QC:39:ILE:HG13  | 2.12                     | 0.49              |
| 3:QC:36:ASP:HA     | 3:QC:39:ILE:HD12  | 1.94                     | 0.49              |
| 11:QK:32:ILE:HD12  | 11:QK:72:ALA:CB   | 2.36                     | 0.49              |
| 12:QL:24:VAL:O     | 12:QL:24:VAL:CG1  | 2.58                     | 0.49              |
| 15:QO:17:ARG:NH1   | 15:QO:77:ARG:CZ   | 2.74                     | 0.49              |
| 16:QP:83:GLU:OE2   | 16:QP:83:GLU:HA   | 2.12                     | 0.49              |
| 22:QV:75:C:H2'     | 22:QV:76:A:O4'    | 2.12                     | 0.49              |
| 25:RA:784:A:O2'    | 25:RA:785:G:H5''  | 2.11                     | 0.49              |
| 25:RA:1006:C:H1'   | 33:RN:106:MET:CE  | 2.41                     | 0.49              |
| 25:RA:2635:C:OP1   | 28:RE:78:LEU:HD12 | 2.11                     | 0.49              |
| 30:RG:103:LEU:HD21 | 30:RG:178:PHE:CZ  | 2.47                     | 0.49              |
| 31:RH:153:LYS:O    | 31:RH:154:PRO:O   | 2.30                     | 0.49              |
| 35:RP:114:ILE:HD11 | 35:RP:130:PHE:HE1 | 1.69                     | 0.49              |
| 40:RU:79:PHE:C     | 40:RU:79:PHE:HD2  | 2.18                     | 0.49              |
| 41:RV:41:GLY:N     | 41:RV:46:VAL:HG13 | 2.26                     | 0.49              |
| 42:RW:29:LEU:HD23  | 42:RW:29:LEU:O    | 2.13                     | 0.49              |
| 44:RY:2:ARG:O      | 44:RY:3:VAL:C     | 2.55                     | 0.49              |
| 50:R4:10:VAL:HG23  | 50:R4:11:PRO:HD2  | 1.93                     | 0.49              |
| 52:R6:20:ASN:O     | 52:R6:21:TYR:CB   | 2.59                     | 0.49              |
| 53:R7:12:ARG:NH1   | 53:R7:12:ARG:HG3  | 2.27                     | 0.49              |
| 53:R7:46:VAL:HG12  | 53:R7:47:ARG:N    | 2.27                     | 0.49              |
| 1:XA:115:G:H4'     | 1:XA:116:A:O5'    | 2.12                     | 0.49              |
| 1:XA:1221:G:OP1    | 19:XS:36:ARG:HD3  | 2.12                     | 0.49              |
| 1:XA:1296:C:H3'    | 1:XA:1297:C:C6    | 2.47                     | 0.49              |
| 1:XA:1346:A:N6     | 7:XG:10:ARG:HD2   | 2.26                     | 0.49              |
| 2:XB:178:ARG:HD2   | 8:XH:71:GLY:HA2   | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:XC:36:ASP:HB3    | 3:XC:40:ARG:NH1    | 2.26                     | 0.49              |
| 3:XC:195:VAL:HG12  | 3:XC:196:LEU:H     | 1.75                     | 0.49              |
| 5:XE:32:VAL:O      | 5:XE:43:LEU:HD12   | 2.12                     | 0.49              |
| 5:XE:126:ARG:HG3   | 5:XE:126:ARG:NH1   | 2.19                     | 0.49              |
| 7:XG:148:ASN:C     | 7:XG:150:ALA:N     | 2.69                     | 0.49              |
| 8:XH:91:ARG:HG2    | 8:XH:91:ARG:NH1    | 2.25                     | 0.49              |
| 9:XI:29:ASN:OD1    | 9:XI:64:THR:HA     | 2.12                     | 0.49              |
| 9:XI:33:PHE:HZ     | 9:XI:47:LEU:HD21   | 1.76                     | 0.49              |
| 13:XM:120:LYS:O    | 13:XM:121:LYS:CB   | 2.60                     | 0.49              |
| 19:XS:68:GLY:HA3   | 50:Y4:68:ARG:CB    | 2.40                     | 0.49              |
| 25:YA:64:A:C5      | 43:YX:66:LEU:HD13  | 2.47                     | 0.49              |
| 25:YA:380:U:H2'    | 25:YA:381:G:H8     | 1.75                     | 0.49              |
| 25:YA:580:C:H2'    | 25:YA:581:C:C6     | 2.47                     | 0.49              |
| 25:YA:2478:A:OP1   | 55:Y9:31:LYS:HD3   | 2.12                     | 0.49              |
| 25:YA:2757:A:N1    | 31:YH:67:LEU:HD22  | 2.27                     | 0.49              |
| 27:YD:76:PRO:HA    | 27:YD:118:VAL:HG23 | 1.93                     | 0.49              |
| 28:YE:37:ARG:HE    | 28:YE:37:ARG:H     | 1.59                     | 0.49              |
| 28:YE:46:ALA:HB1   | 28:YE:80:GLU:HB2   | 1.94                     | 0.49              |
| 29:YF:11:VAL:CG1   | 29:YF:12:LEU:N     | 2.75                     | 0.49              |
| 30:YG:49:ASP:OD1   | 30:YG:51:ARG:HG3   | 2.12                     | 0.49              |
| 30:YG:114:ILE:HG21 | 30:YG:117:PHE:HB2  | 1.93                     | 0.49              |
| 33:YN:137:LYS:HG3  | 33:YN:138:LEU:H    | 1.77                     | 0.49              |
| 34:YO:47:ILE:CG1   | 34:YO:48:PRO:HD2   | 2.42                     | 0.49              |
| 44:YY:16:ALA:O     | 44:YY:21:LYS:HD3   | 2.11                     | 0.49              |
| 48:Y2:69:ARG:CB    | 48:Y2:69:ARG:HH11  | 2.25                     | 0.49              |
| 50:Y4:9:LEU:H      | 50:Y4:27:THR:CG2   | 2.25                     | 0.49              |
| 1:QA:972:C:H4'     | 10:QJ:57:LYS:HG3   | 1.93                     | 0.49              |
| 1:QA:1055:A:N7     | 1:QA:1200:C:N4     | 2.61                     | 0.49              |
| 3:QC:178:LEU:N     | 3:QC:178:LEU:HD22  | 2.27                     | 0.49              |
| 4:QD:150:GLU:C     | 4:QD:152:SER:H     | 2.20                     | 0.49              |
| 9:QI:83:ARG:C      | 9:QI:86:VAL:HG12   | 2.36                     | 0.49              |
| 16:QP:39:TYR:CE2   | 16:QP:41:PRO:HD3   | 2.48                     | 0.49              |
| 25:RA:389:G:H1     | 35:RP:70:GLN:HB3   | 1.77                     | 0.49              |
| 25:RA:513:A:H5'    | 25:RA:1216:G:O2'   | 2.12                     | 0.49              |
| 26:RB:80:U:O2'     | 26:RB:81:G:H5''    | 2.12                     | 0.49              |
| 27:RD:123:ALA:HB3  | 27:RD:131:LEU:HG   | 1.94                     | 0.49              |
| 31:RH:128:PRO:HD2  | 31:RH:129:THR:N    | 2.25                     | 0.49              |
| 33:RN:73:THR:HG22  | 33:RN:82:LEU:HD11  | 1.93                     | 0.49              |
| 35:RP:88:LEU:C     | 35:RP:88:LEU:HD23  | 2.37                     | 0.49              |
| 40:RU:53:ARG:C     | 40:RU:55:ARG:H     | 2.19                     | 0.49              |
| 43:RX:47:PHE:O     | 43:RX:48:LYS:C     | 2.55                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:RX:70:LEU:N     | 43:RX:70:LEU:CD2  | 2.71                     | 0.49              |
| 44:RY:81:LYS:HD3   | 44:RY:97:ARG:HD3  | 1.94                     | 0.49              |
| 45:RZ:45:ASP:OD1   | 45:RZ:49:ARG:NE   | 2.38                     | 0.49              |
| 49:R3:7:LYS:CB     | 49:R3:34:GLU:HG2  | 2.41                     | 0.49              |
| 1:XA:58:C:O2'      | 1:XA:388:G:N7     | 2.38                     | 0.49              |
| 1:XA:819:A:H8      | 1:XA:819:A:H5'    | 1.77                     | 0.49              |
| 2:XB:172:ILE:H     | 2:XB:172:ILE:CD1  | 2.18                     | 0.49              |
| 5:XE:41:VAL:CG1    | 5:XE:112:LEU:O    | 2.60                     | 0.49              |
| 7:XG:50:ILE:HG21   | 7:XG:58:PRO:HA    | 1.93                     | 0.49              |
| 8:XH:84:ARG:O      | 8:XH:135:CYS:HB2  | 2.12                     | 0.49              |
| 8:XH:91:ARG:HH11   | 8:XH:91:ARG:CG    | 2.22                     | 0.49              |
| 17:XQ:33:GLY:O     | 17:XQ:34:LYS:C    | 2.55                     | 0.49              |
| 25:YA:71:A:N6      | 25:YA:114:U:H1'   | 2.27                     | 0.49              |
| 25:YA:858:U:H1'    | 25:YA:2268:A:H2'  | 1.94                     | 0.49              |
| 25:YA:1250:G:OP2   | 35:YP:21:ARG:HD3  | 2.13                     | 0.49              |
| 25:YA:1972:A:H2'   | 25:YA:1973:G:C8   | 2.47                     | 0.49              |
| 25:YA:2012:G:H4'   | 42:YW:96:ILE:HD11 | 1.93                     | 0.49              |
| 30:YG:83:ARG:HH11  | 30:YG:83:ARG:HG2  | 1.76                     | 0.49              |
| 34:YO:69:ILE:O     | 34:YO:76:ALA:HA   | 2.12                     | 0.49              |
| 35:YP:112:LEU:HD22 | 35:YP:113:LYS:N   | 2.26                     | 0.49              |
| 36:YQ:2:LEU:HD23   | 36:YQ:2:LEU:N     | 2.27                     | 0.49              |
| 36:YQ:29:PHE:N     | 36:YQ:105:GLU:OE2 | 2.41                     | 0.49              |
| 38:YS:52:SER:O     | 38:YS:56:LEU:CD2  | 2.60                     | 0.49              |
| 39:YT:57:PHE:O     | 39:YT:58:ASN:C    | 2.53                     | 0.49              |
| 44:YY:44:ILE:CG1   | 44:YY:45:VAL:H    | 2.24                     | 0.49              |
| 47:Y1:93:GLU:O     | 47:Y1:97:LEU:HD11 | 2.12                     | 0.49              |
| 50:Y4:38:LYS:C     | 50:Y4:40:HIS:H    | 2.07                     | 0.49              |
| 1:QA:35:G:H2'      | 1:QA:36:C:C6      | 2.47                     | 0.49              |
| 1:QA:974:A:H1'     | 14:QN:31:ARG:HE   | 1.76                     | 0.49              |
| 1:QA:1213:A:N6     | 1:QA:1215:G:N3    | 2.60                     | 0.49              |
| 4:QD:166:LYS:HG3   | 27:YD:135:PHE:HZ  | 1.76                     | 0.49              |
| 5:QE:32:VAL:O      | 5:QE:43:LEU:HD12  | 2.12                     | 0.49              |
| 5:QE:36:ASP:C      | 5:QE:37:ARG:HG2   | 2.38                     | 0.49              |
| 7:QG:148:ASN:C     | 7:QG:150:ALA:N    | 2.69                     | 0.49              |
| 9:QI:83:ARG:HA     | 9:QI:86:VAL:CG1   | 2.41                     | 0.49              |
| 13:QM:14:ARG:HG3   | 13:QM:16:ASP:OD2  | 2.12                     | 0.49              |
| 20:QT:10:LEU:C     | 20:QT:12:ALA:H    | 2.20                     | 0.49              |
| 21:QU:6:ARG:HE     | 21:QU:15:ARG:NH2  | 2.09                     | 0.49              |
| 21:QU:6:ARG:HH21   | 21:QU:15:ARG:NE   | 2.09                     | 0.49              |
| 21:QU:6:ARG:C      | 21:QU:8:THR:H     | 2.20                     | 0.49              |
| 25:RA:900:A:H3'    | 25:RA:901:A:C8    | 2.44                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:928:G:O2'   | 49:R3:43:ILE:HD11  | 2.12                     | 0.49              |
| 25:RA:1869:G:H5'  | 25:RA:1870:C:OP2   | 2.12                     | 0.49              |
| 25:RA:2392:A:H8   | 35:RP:60:MET:HG3   | 1.72                     | 0.49              |
| 27:RD:10:THR:HG23 | 27:RD:13:ARG:CB    | 2.34                     | 0.49              |
| 27:RD:35:LYS:CG   | 27:RD:64:ILE:HG22  | 2.42                     | 0.49              |
| 28:RE:23:VAL:HG12 | 28:RE:173:VAL:HG21 | 1.94                     | 0.49              |
| 30:RG:83:ARG:HG2  | 30:RG:83:ARG:HH11  | 1.76                     | 0.49              |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:CG2   | 2.41                     | 0.49              |
| 33:RN:118:LYS:C   | 33:RN:120:LEU:H    | 2.21                     | 0.49              |
| 35:RP:31:ALA:C    | 35:RP:32:THR:CG2   | 2.85                     | 0.49              |
| 35:RP:147:LEU:O   | 35:RP:148:LEU:HB2  | 2.11                     | 0.49              |
| 37:RR:118:GLU:OXT | 37:RR:118:GLU:HG3  | 2.11                     | 0.49              |
| 50:R4:9:LEU:H     | 50:R4:27:THR:CG2   | 2.25                     | 0.49              |
| 50:R4:57:GLU:O    | 50:R4:61:ARG:O     | 2.30                     | 0.49              |
| 3:XC:35:GLU:O     | 3:XC:39:ILE:HG13   | 2.13                     | 0.49              |
| 3:XC:42:LEU:HD12  | 3:XC:45:LYS:HZ3    | 1.76                     | 0.49              |
| 8:XH:83:ILE:HB    | 8:XH:137:VAL:HG13  | 1.94                     | 0.49              |
| 8:XH:109:ILE:HG12 | 8:XH:110:ALA:N     | 2.27                     | 0.49              |
| 9:XI:5:TYR:HA     | 9:XI:17:VAL:O      | 2.12                     | 0.49              |
| 16:XP:59:TRP:HA   | 16:XP:59:TRP:HE3   | 1.76                     | 0.49              |
| 17:XQ:3:LYS:HD2   | 17:XQ:60:ILE:HD11  | 1.95                     | 0.49              |
| 20:XT:26:ASN:CB   | 20:XT:71:THR:HG23  | 2.43                     | 0.49              |
| 21:XU:2:GLY:O     | 21:XU:4:GLY:N      | 2.45                     | 0.49              |
| 25:YA:1196:C:HO2' | 25:YA:1228:G:HO2'  | 1.60                     | 0.49              |
| 25:YA:1265:A:H8   | 25:YA:1265:A:OP1   | 1.94                     | 0.49              |
| 25:YA:2572:A:C8   | 28:YE:144:ARG:HB3  | 2.47                     | 0.49              |
| 27:YD:2:ALA:CB    | 27:YD:20:ASP:HB3   | 2.42                     | 0.49              |
| 28:YE:61:ARG:CB   | 28:YE:62:PRO:CD    | 2.90                     | 0.49              |
| 30:YG:121:ASN:C   | 30:YG:123:ASN:H    | 2.20                     | 0.49              |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:HG23  | 1.93                     | 0.49              |
| 33:YN:6:PRO:HG2   | 33:YN:43:THR:OG1   | 2.11                     | 0.49              |
| 33:YN:73:THR:CG2  | 33:YN:82:LEU:HD11  | 2.43                     | 0.49              |
| 35:YP:81:GLN:CD   | 35:YP:106:LEU:O    | 2.55                     | 0.49              |
| 38:YS:89:ARG:O    | 38:YS:90:GLY:C     | 2.54                     | 0.49              |
| 38:YS:99:LYS:O    | 38:YS:101:LEU:N    | 2.45                     | 0.49              |
| 40:YU:92:ARG:NH1  | 40:YU:95:LEU:HD11  | 2.26                     | 0.49              |
| 42:YW:28:SER:C    | 42:YW:30:GLU:N     | 2.69                     | 0.49              |
| 42:YW:51:LEU:HD23 | 42:YW:105:VAL:HG11 | 1.94                     | 0.49              |
| 45:YZ:5:LEU:HD23  | 45:YZ:47:VAL:HG21  | 1.94                     | 0.49              |
| 47:Y1:8:SER:HB3   | 47:Y1:66:HIS:CE1   | 2.47                     | 0.49              |
| 47:Y1:19:GLN:OE1  | 47:Y1:19:GLN:HA    | 2.12                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:Y1:40:ARG:NH2   | 47:Y1:42:GLN:HG2  | 2.27                     | 0.49              |
| 47:Y1:67:ILE:N     | 47:Y1:68:PRO:CD   | 2.76                     | 0.49              |
| 49:Y3:21:ALA:O     | 49:Y3:25:ALA:N    | 2.41                     | 0.49              |
| 52:Y6:44:ARG:O     | 52:Y6:45:LYS:CB   | 2.60                     | 0.49              |
| 54:Y8:10:ALA:O     | 54:Y8:14:VAL:HG12 | 2.11                     | 0.49              |
| 1:QA:643:C:H2'     | 1:QA:644:G:H8     | 1.77                     | 0.49              |
| 1:QA:677:U:H1'     | 11:QK:119:CYS:SG  | 2.53                     | 0.49              |
| 1:QA:719:C:O2'     | 18:QR:49:LYS:HB3  | 2.12                     | 0.49              |
| 1:QA:966:G:O2'     | 9:QI:127:LYS:O    | 2.31                     | 0.49              |
| 4:QD:23:GLY:H      | 4:QD:26:CYS:HB2   | 1.77                     | 0.49              |
| 4:QD:206:PHE:HD2   | 4:QD:207:TYR:CE1  | 2.31                     | 0.49              |
| 5:QE:11:ILE:CG1    | 5:QE:31:LEU:HD12  | 2.42                     | 0.49              |
| 5:QE:82:VAL:HG12   | 5:QE:83:GLU:H     | 1.78                     | 0.49              |
| 8:QH:29:SER:CB     | 8:QH:32:LYS:HG3   | 2.28                     | 0.49              |
| 14:QN:8:GLU:O      | 14:QN:10:ALA:N    | 2.45                     | 0.49              |
| 20:QT:37:SER:O     | 20:QT:41:ILE:HG12 | 2.12                     | 0.49              |
| 25:RA:270(F):U:H2' | 25:RA:270(G):C:C6 | 2.47                     | 0.49              |
| 25:RA:270(S):G:H1' | 47:R1:78:LYS:HD2  | 1.94                     | 0.49              |
| 25:RA:686:G:N2     | 25:RA:788:A:H61   | 2.10                     | 0.49              |
| 25:RA:1152:C:H2'   | 25:RA:1153:C:H6   | 1.77                     | 0.49              |
| 25:RA:1426:G:OP2   | 25:RA:1427:A:O2'  | 2.27                     | 0.49              |
| 25:RA:2776:A:OP1   | 25:RA:2776:A:H3'  | 2.12                     | 0.49              |
| 27:RD:12:SER:C     | 27:RD:14:ARG:N    | 2.70                     | 0.49              |
| 27:RD:25:THR:O     | 27:RD:27:THR:HG22 | 2.12                     | 0.49              |
| 27:RD:241:PRO:O    | 27:RD:242:ARG:C   | 2.55                     | 0.49              |
| 30:RG:49:ASP:OD1   | 30:RG:51:ARG:HG3  | 2.12                     | 0.49              |
| 31:RH:23:ARG:HD2   | 31:RH:34:GLU:OE2  | 2.12                     | 0.49              |
| 31:RH:120:GLY:HA3  | 31:RH:140:LYS:NZ  | 2.28                     | 0.49              |
| 32:RI:8:PRO:HD3    | 32:RI:15:VAL:HG13 | 1.94                     | 0.49              |
| 35:RP:49:ARG:HE    | 54:R8:59:LYS:HG2  | 1.76                     | 0.49              |
| 36:RQ:90:VAL:C     | 36:RQ:92:GLY:N    | 2.70                     | 0.49              |
| 37:RR:67:LEU:HD13  | 37:RR:76:VAL:CG2  | 2.27                     | 0.49              |
| 40:RU:79:PHE:HE2   | 40:RU:83:LEU:HD22 | 1.78                     | 0.49              |
| 41:RV:76:LYS:HG3   | 41:RV:81:TYR:CD1  | 2.48                     | 0.49              |
| 44:RY:77:PRO:O     | 44:RY:78:ALA:HB2  | 2.11                     | 0.49              |
| 50:R4:22:ILE:HD12  | 50:R4:22:ILE:H    | 1.77                     | 0.49              |
| 1:XA:186:C:H2'     | 1:XA:186(A):C:H6  | 1.78                     | 0.49              |
| 1:XA:1118:C:OP1    | 9:XI:9:ARG:HD3    | 2.13                     | 0.49              |
| 1:XA:1204:A:OP1    | 14:YN:3:ARG:NH2   | 2.45                     | 0.49              |
| 2:XB:68:ILE:O      | 2:XB:91:PRO:HD2   | 2.13                     | 0.49              |
| 4:XD:118:ARG:NH2   | 4:XD:136:PRO:HB2  | 2.28                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:XI:43:ALA:HA     | 9:XI:74:ILE:HD13   | 1.94                     | 0.49              |
| 9:XI:113:LYS:H     | 9:XI:119:ALA:HA    | 1.77                     | 0.49              |
| 10:XJ:22:LYS:NZ    | 10:XJ:23:ILE:HG12  | 2.28                     | 0.49              |
| 13:XM:90:LEU:HA    | 13:XM:93:ARG:CD    | 2.34                     | 0.49              |
| 14:XN:8:GLU:O      | 14:XN:10:ALA:N     | 2.45                     | 0.49              |
| 20:XT:10:LEU:C     | 20:XT:12:ALA:H     | 2.21                     | 0.49              |
| 21:XU:6:ARG:C      | 21:XU:8:THR:H      | 2.20                     | 0.49              |
| 25:YA:71:A:H2      | 43:YX:31:HIS:HE2   | 1.59                     | 0.49              |
| 25:YA:746:A:C6     | 25:YA:2611:U:H5''  | 2.48                     | 0.49              |
| 25:YA:1101:U:H2'   | 25:YA:1102:C:C6    | 2.48                     | 0.49              |
| 25:YA:1217:C:OP1   | 40:YU:15:LYS:NZ    | 2.31                     | 0.49              |
| 25:YA:2545:G:H2'   | 25:YA:2546:U:O4'   | 2.12                     | 0.49              |
| 25:YA:2610:C:H4'   | 25:YA:2611:U:OP2   | 2.11                     | 0.49              |
| 27:YD:2:ALA:CB     | 27:YD:20:ASP:CB    | 2.90                     | 0.49              |
| 28:YE:18:ASP:O     | 28:YE:19:ARG:C     | 2.56                     | 0.49              |
| 31:YH:103:LEU:H    | 31:YH:103:LEU:HD23 | 1.77                     | 0.49              |
| 33:YN:46:VAL:O     | 33:YN:47:ALA:CB    | 2.57                     | 0.49              |
| 33:YN:82:LEU:HD12  | 33:YN:83:LYS:N     | 2.27                     | 0.49              |
| 35:YP:36:LYS:HB2   | 35:YP:40:SER:HB3   | 1.94                     | 0.49              |
| 40:YU:81:HIS:CE1   | 40:YU:117:GLN:HG3  | 2.48                     | 0.49              |
| 41:YV:3:ALA:HB3    | 41:YV:14:VAL:HG23  | 1.93                     | 0.49              |
| 42:YW:29:LEU:O     | 42:YW:29:LEU:HD23  | 2.13                     | 0.49              |
| 44:YY:81:LYS:CD    | 44:YY:97:ARG:HE    | 2.20                     | 0.49              |
| 50:Y4:36:CYS:O     | 50:Y4:39:CYS:CB    | 2.55                     | 0.49              |
| 2:QB:181:PHE:O     | 2:QB:183:PRO:HD3   | 2.12                     | 0.49              |
| 4:QD:30:LYS:CG     | 4:QD:35:ARG:NE     | 2.64                     | 0.49              |
| 4:QD:166:LYS:HD3   | 27:YD:188:GLU:OE2  | 2.12                     | 0.49              |
| 6:QF:101:ALA:HA    | 18:QR:28:GLU:HG2   | 1.95                     | 0.49              |
| 8:QH:82:HIS:CD2    | 8:QH:82:HIS:C      | 2.91                     | 0.49              |
| 11:QK:29:ILE:HG13  | 11:QK:44:SER:HB3   | 1.93                     | 0.49              |
| 15:QO:77:ARG:HA    | 15:QO:80:ALA:HB3   | 1.95                     | 0.49              |
| 25:RA:957:A:N1     | 25:RA:2458:G:H4'   | 2.27                     | 0.49              |
| 25:RA:975:G:H1'    | 25:RA:990:A:C2     | 2.46                     | 0.49              |
| 25:RA:1091:G:N2    | 25:RA:1101:U:H1'   | 2.27                     | 0.49              |
| 25:RA:1113:U:OP1   | 31:RH:2:SER:N      | 2.45                     | 0.49              |
| 25:RA:1794:U:H2'   | 25:RA:1795:C:H6    | 1.76                     | 0.49              |
| 26:RB:29:A:OP2     | 38:RS:32:LEU:HG    | 2.12                     | 0.49              |
| 28:RE:119:ARG:HD3  | 28:RE:160:TYR:HD2  | 1.78                     | 0.49              |
| 31:RH:103:LEU:HD23 | 31:RH:103:LEU:H    | 1.77                     | 0.49              |
| 34:RO:69:ILE:O     | 34:RO:76:ALA:HA    | 2.12                     | 0.49              |
| 34:RO:105:GLU:O    | 34:RO:108:GLU:HB2  | 2.12                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:RQ:132:VAL:HG12 | 36:RQ:133:ARG:N   | 2.27                     | 0.49              |
| 37:RR:10:LEU:O     | 37:RR:11:ASN:C    | 2.55                     | 0.49              |
| 41:RV:7:THR:HG23   | 41:RV:22:VAL:HG11 | 1.94                     | 0.49              |
| 44:RY:35:TYR:CD1   | 44:RY:69:ALA:HB3  | 2.48                     | 0.49              |
| 47:R1:67:ILE:N     | 47:R1:68:PRO:CD   | 2.76                     | 0.49              |
| 47:R1:73:LEU:C     | 47:R1:75:GLU:N    | 2.70                     | 0.49              |
| 48:R2:41:ILE:HD11  | 48:R2:44:LEU:CB   | 2.42                     | 0.49              |
| 50:R4:42:PHE:O     | 50:R4:44:THR:O    | 2.31                     | 0.49              |
| 52:R6:37:ARG:HA    | 52:R6:37:ARG:HE   | 1.77                     | 0.49              |
| 54:R8:15:LYS:HD3   | 54:R8:15:LYS:C    | 2.37                     | 0.49              |
| 1:XA:554:C:H2'     | 1:XA:555:C:C6     | 2.48                     | 0.49              |
| 1:XA:692:U:H5      | 11:XK:26:ASN:OD1  | 1.96                     | 0.49              |
| 1:XA:976:G:H5''    | 1:XA:1358:U:O2'   | 2.11                     | 0.49              |
| 2:XB:15:VAL:H      | 2:XB:16:HIS:CE1   | 2.30                     | 0.49              |
| 2:XB:207:ALA:O     | 2:XB:209:ARG:N    | 2.45                     | 0.49              |
| 3:XC:178:LEU:N     | 3:XC:178:LEU:HD22 | 2.28                     | 0.49              |
| 4:XD:68:TYR:O      | 4:XD:69:GLY:C     | 2.55                     | 0.49              |
| 4:XD:198:VAL:HG12  | 4:XD:199:ASN:H    | 1.74                     | 0.49              |
| 9:XI:110:GLU:O     | 9:XI:110:GLU:HG3  | 2.12                     | 0.49              |
| 13:XM:66:LEU:C     | 13:XM:70:LEU:HB2  | 2.37                     | 0.49              |
| 13:XM:120:LYS:O    | 13:XM:121:LYS:HB2 | 2.10                     | 0.49              |
| 25:YA:580:C:H2'    | 25:YA:581:C:H6    | 1.77                     | 0.49              |
| 25:YA:1403:C:H5''  | 25:YA:1471:A:C1'  | 2.42                     | 0.49              |
| 25:YA:1657:C:H2'   | 25:YA:1658:C:C6   | 2.48                     | 0.49              |
| 25:YA:2277:G:P     | 36:YQ:85:LYS:HB2  | 2.53                     | 0.49              |
| 30:YG:107:LEU:HD11 | 30:YG:178:PHE:CD1 | 2.48                     | 0.49              |
| 33:YN:129:PRO:C    | 33:YN:131:GLN:H   | 2.20                     | 0.49              |
| 34:YO:1:MET:HE3    | 34:YO:67:LYS:HG2  | 1.95                     | 0.49              |
| 39:YT:38:ASN:O     | 39:YT:39:ARG:O    | 2.30                     | 0.49              |
| 39:YT:57:PHE:O     | 39:YT:59:THR:N    | 2.46                     | 0.49              |
| 50:Y4:47:GLN:O     | 50:Y4:48:ARG:CB   | 2.60                     | 0.49              |
| 53:Y7:46:VAL:HG12  | 53:Y7:47:ARG:N    | 2.27                     | 0.49              |
| 54:Y8:16:ILE:CD1   | 54:Y8:57:ARG:HG2  | 2.42                     | 0.49              |
| 55:Y9:1:MET:HE1    | 55:Y9:32:HIS:HD2  | 1.77                     | 0.49              |
| 1:QA:520:A:N1      | 1:QA:536:C:H1'    | 2.27                     | 0.49              |
| 1:QA:1218:C:H2'    | 1:QA:1219:U:C6    | 2.47                     | 0.49              |
| 2:QB:103:THR:N     | 2:QB:180:LEU:HD11 | 2.27                     | 0.49              |
| 13:QM:120:LYS:O    | 13:QM:121:LYS:CB  | 2.60                     | 0.49              |
| 16:QP:43:LYS:HE2   | 16:QP:48:TRP:CZ3  | 2.47                     | 0.49              |
| 17:QQ:74:LEU:HD12  | 17:QQ:75:ARG:NE   | 2.28                     | 0.49              |
| 23:QY:40:G:H2'     | 23:QY:41:A:H5'    | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:25:U:H5''    | 42:RW:80:PRO:HD3   | 1.94                     | 0.49              |
| 25:RA:229:A:OP1    | 25:RA:229:A:H4'    | 2.11                     | 0.49              |
| 25:RA:2114:A:N6    | 25:RA:2119:A:H62   | 2.11                     | 0.49              |
| 25:RA:2232:U:OP1   | 47:R1:40:ARG:NH1   | 2.45                     | 0.49              |
| 25:RA:2306:C:H2'   | 25:RA:2307:G:N2    | 2.27                     | 0.49              |
| 27:RD:69:ARG:C     | 27:RD:71:ASP:N     | 2.69                     | 0.49              |
| 27:RD:182:LEU:H    | 27:RD:272:ALA:CB   | 2.25                     | 0.49              |
| 28:RE:55:ASN:O     | 28:RE:57:LYS:N     | 2.45                     | 0.49              |
| 30:RG:107:LEU:HD11 | 30:RG:178:PHE:CD1  | 2.48                     | 0.49              |
| 31:RH:7:LEU:C      | 31:RH:7:LEU:HD12   | 2.37                     | 0.49              |
| 33:RN:120:LEU:HD11 | 33:RN:122:VAL:CG2  | 2.42                     | 0.49              |
| 34:RO:8:LEU:N      | 34:RO:8:LEU:CD2    | 2.76                     | 0.49              |
| 36:RQ:29:PHE:N     | 36:RQ:105:GLU:OE2  | 2.41                     | 0.49              |
| 38:RS:18:ILE:O     | 38:RS:19:LYS:O     | 2.31                     | 0.49              |
| 40:RU:92:ARG:CD    | 40:RU:94:ASN:HB3   | 2.42                     | 0.49              |
| 43:RX:51:VAL:HG13  | 43:RX:81:VAL:HG23  | 1.93                     | 0.49              |
| 44:RY:84:ARG:HD3   | 44:RY:86:ARG:NH1   | 2.28                     | 0.49              |
| 47:R1:40:ARG:NH2   | 47:R1:42:GLN:HG2   | 2.27                     | 0.49              |
| 48:R2:33:MET:O     | 48:R2:37:PHE:HD1   | 1.95                     | 0.49              |
| 53:R7:9:ARG:HH12   | 53:R7:47:ARG:HG3   | 1.76                     | 0.49              |
| 1:XA:1130:A:N6     | 1:XA:1131:G:O6     | 2.45                     | 0.49              |
| 1:XA:1305:G:OP1    | 21:XU:2:GLY:HA2    | 2.13                     | 0.49              |
| 1:XA:1493:A:OP1    | 58:XA:1675:PAR:H51 | 2.13                     | 0.49              |
| 2:XB:95:GLN:NE2    | 2:XB:147:LYS:HE2   | 2.27                     | 0.49              |
| 4:XD:9:CYS:SG      | 4:XD:22:LYS:CD     | 2.98                     | 0.49              |
| 6:XF:101:ALA:HA    | 18:XR:28:GLU:HG2   | 1.95                     | 0.49              |
| 8:XH:14:ARG:O      | 8:XH:14:ARG:HG2    | 2.12                     | 0.49              |
| 8:XH:61:VAL:HG12   | 8:XH:63:LEU:HD13   | 1.94                     | 0.49              |
| 19:XS:9:VAL:O      | 19:XS:10:PHE:HB3   | 2.13                     | 0.49              |
| 23:XY:36:G:H1      | 24:XX:4:C:H42      | 1.60                     | 0.49              |
| 25:YA:636:G:OP1    | 35:YP:132:LYS:HB2  | 2.13                     | 0.49              |
| 26:YB:43:C:H5'     | 50:Y4:1:MET:HA     | 1.95                     | 0.49              |
| 27:YD:35:LYS:CG    | 27:YD:64:ILE:HG22  | 2.42                     | 0.49              |
| 27:YD:227:ASN:HB3  | 27:YD:228:PRO:CD   | 2.30                     | 0.49              |
| 28:YE:17:ASP:N     | 28:YE:17:ASP:OD2   | 2.46                     | 0.49              |
| 29:YF:144:LYS:C    | 29:YF:146:ALA:H    | 2.21                     | 0.49              |
| 31:YH:153:LYS:O    | 31:YH:154:PRO:O    | 2.30                     | 0.49              |
| 33:YN:95:PRO:O     | 33:YN:97:ARG:N     | 2.46                     | 0.49              |
| 34:YO:20:MET:HG2   | 34:YO:21:CYS:O     | 2.11                     | 0.49              |
| 37:YR:1:MET:O      | 37:YR:2:ARG:CB     | 2.60                     | 0.49              |
| 38:YS:60:GLY:O     | 38:YS:61:ASN:CB    | 2.55                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:YT:39:ARG:CG   | 39:YT:40:THR:H    | 2.22                     | 0.49              |
| 41:YV:29:PRO:O    | 41:YV:61:VAL:HG22 | 2.12                     | 0.49              |
| 44:YY:84:ARG:HD3  | 44:YY:86:ARG:NH1  | 2.28                     | 0.49              |
| 52:Y6:7:ILE:C     | 52:Y6:9:LEU:N     | 2.65                     | 0.49              |
| 54:Y8:58:ILE:O    | 54:Y8:61:LEU:HD12 | 2.13                     | 0.49              |
| 1:QA:446:G:H1     | 1:QA:488:C:H42    | 1.61                     | 0.49              |
| 1:QA:501:C:OP1    | 12:QL:117:ARG:NH2 | 2.42                     | 0.49              |
| 1:QA:546:G:P      | 4:QD:72:GLU:HB3   | 2.53                     | 0.49              |
| 1:QA:690:G:H22    | 11:QK:55:LYS:NZ   | 2.10                     | 0.49              |
| 3:QC:173:VAL:N    | 3:QC:174:PRO:HD3  | 2.28                     | 0.49              |
| 4:QD:3:ARG:O      | 4:QD:4:TYR:C      | 2.55                     | 0.49              |
| 4:QD:9:CYS:SG     | 4:QD:22:LYS:CE    | 3.01                     | 0.49              |
| 4:QD:9:CYS:SG     | 4:QD:22:LYS:CD    | 2.98                     | 0.49              |
| 6:QF:51:PRO:HA    | 6:QF:55:ASP:O     | 2.13                     | 0.49              |
| 7:QG:40:ALA:O     | 7:QG:41:ARG:C     | 2.55                     | 0.49              |
| 9:QI:110:GLU:O    | 9:QI:110:GLU:HG3  | 2.12                     | 0.49              |
| 10:QJ:16:LEU:HD13 | 10:QJ:16:LEU:C    | 2.38                     | 0.49              |
| 11:QK:110:ASP:HB2 | 18:QR:88:LYS:HD3  | 1.95                     | 0.49              |
| 14:QN:8:GLU:C     | 14:QN:10:ALA:N    | 2.68                     | 0.49              |
| 15:QO:54:ARG:O    | 15:QO:55:GLY:C    | 2.55                     | 0.49              |
| 20:QT:60:GLU:HG3  | 20:QT:81:LYS:HE3  | 1.94                     | 0.49              |
| 20:QT:83:ARG:C    | 20:QT:86:ARG:HB3  | 2.38                     | 0.49              |
| 20:QT:97:ALA:HB3  | 20:QT:99:LEU:CD1  | 2.43                     | 0.49              |
| 25:RA:277:C:H4'   | 25:RA:278:A:OP2   | 2.11                     | 0.49              |
| 25:RA:821:A:H2'   | 25:RA:946:G:H5''  | 1.94                     | 0.49              |
| 25:RA:1085:A:O2'  | 25:RA:1086:A:OP1  | 2.25                     | 0.49              |
| 25:RA:1549:C:O2'  | 25:RA:1733:G:N2   | 2.45                     | 0.49              |
| 25:RA:2284:C:C5   | 52:R6:27:LYS:HE2  | 2.48                     | 0.49              |
| 27:RD:198:ASN:C   | 27:RD:198:ASN:ND2 | 2.69                     | 0.49              |
| 28:RE:95:ILE:H    | 28:RE:95:ILE:CD1  | 2.18                     | 0.49              |
| 30:RG:113:ARG:HD2 | 50:R4:33:VAL:CG1  | 2.43                     | 0.49              |
| 31:RH:54:ARG:HD3  | 31:RH:65:HIS:ND1  | 2.27                     | 0.49              |
| 31:RH:98:LEU:HD12 | 31:RH:102:ALA:O   | 2.13                     | 0.49              |
| 33:RN:30:ILE:O    | 33:RN:34:LEU:HD23 | 2.13                     | 0.49              |
| 33:RN:95:PRO:O    | 33:RN:97:ARG:N    | 2.46                     | 0.49              |
| 36:RQ:23:GLY:O    | 36:RQ:24:GLY:O    | 2.30                     | 0.49              |
| 37:RR:71:GLN:HA   | 37:RR:71:GLN:HE21 | 1.77                     | 0.49              |
| 39:RT:16:ARG:NE   | 39:RT:19:LEU:HD21 | 2.28                     | 0.49              |
| 42:RW:30:GLU:O    | 42:RW:34:ASN:ND2  | 2.46                     | 0.49              |
| 54:R8:33:ASN:O    | 54:R8:35:GLN:N    | 2.46                     | 0.49              |
| 1:XA:67:C:H2'     | 1:XA:68:G:H8      | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:201:C:H42    | 1:XA:216:G:H1     | 1.60                     | 0.49              |
| 1:XA:474:G:H2'    | 1:XA:475:G:C8     | 2.48                     | 0.49              |
| 1:XA:836:G:C6     | 1:XA:851:G:C6     | 3.00                     | 0.49              |
| 1:XA:950:U:H2'    | 1:XA:951:G:C8     | 2.47                     | 0.49              |
| 1:XA:1298:C:O2'   | 1:XA:1299:A:OP2   | 2.28                     | 0.49              |
| 3:XC:188:LEU:N    | 3:XC:188:LEU:CD2  | 2.76                     | 0.49              |
| 6:XF:72:VAL:HG13  | 6:XF:73:ASN:N     | 2.27                     | 0.49              |
| 11:XK:53:SER:C    | 11:XK:55:LYS:H    | 2.21                     | 0.49              |
| 16:XP:83:GLU:HA   | 16:XP:83:GLU:OE2  | 2.12                     | 0.49              |
| 25:YA:1803:A:N6   | 25:YA:1814:G:O2'  | 2.34                     | 0.49              |
| 27:YD:30:GLU:CD   | 27:YD:63:ARG:HE   | 2.21                     | 0.49              |
| 28:YE:179:GLU:O   | 28:YE:180:ASN:HB2 | 2.12                     | 0.49              |
| 29:YF:51:THR:O    | 29:YF:93:LYS:NZ   | 2.38                     | 0.49              |
| 31:YH:98:LEU:HD12 | 31:YH:102:ALA:O   | 2.13                     | 0.49              |
| 39:YT:135:ALA:C   | 39:YT:137:LYS:N   | 2.71                     | 0.49              |
| 43:YX:51:VAL:HG13 | 43:YX:81:VAL:HG23 | 1.93                     | 0.49              |
| 44:YY:88:LYS:NZ   | 44:YY:88:LYS:HA   | 2.27                     | 0.49              |
| 44:YY:95:LYS:N    | 44:YY:95:LYS:CD   | 2.75                     | 0.49              |
| 50:Y4:1:MET:HG3   | 50:Y4:1:MET:O     | 2.12                     | 0.49              |
| 51:Y5:2:ALA:O     | 51:Y5:3:LYS:CB    | 2.60                     | 0.49              |
| 55:Y9:7:VAL:HG12  | 55:Y9:25:VAL:HG21 | 1.94                     | 0.49              |
| 1:QA:481:G:O2'    | 1:QA:482:A:O5'    | 2.31                     | 0.49              |
| 1:QA:1297:C:O2'   | 1:QA:1298:C:O5'   | 2.31                     | 0.49              |
| 4:QD:30:LYS:HD2   | 4:QD:35:ARG:HH21  | 1.78                     | 0.49              |
| 5:QE:41:VAL:CG1   | 5:QE:112:LEU:O    | 2.60                     | 0.49              |
| 9:QI:18:PHE:O     | 9:QI:61:ALA:HA    | 2.13                     | 0.49              |
| 9:QI:79:LEU:O     | 9:QI:79:LEU:HD13  | 2.13                     | 0.49              |
| 10:QJ:33:GLN:HB2  | 10:QJ:75:ILE:CD1  | 2.43                     | 0.49              |
| 13:QM:4:ILE:HG22  | 13:QM:5:ALA:H     | 1.75                     | 0.49              |
| 13:QM:66:LEU:C    | 13:QM:70:LEU:HB2  | 2.38                     | 0.49              |
| 13:QM:102:ARG:O   | 13:QM:102:ARG:HG3 | 2.12                     | 0.49              |
| 20:QT:53:LEU:HA   | 20:QT:56:MET:CB   | 2.43                     | 0.49              |
| 25:RA:507:A:H5''  | 25:RA:508:G:H5'   | 1.94                     | 0.49              |
| 25:RA:1695:G:H1'  | 27:RD:8:PRO:O     | 2.12                     | 0.49              |
| 25:RA:2052:G:H4'  | 28:RE:143:ASN:O   | 2.13                     | 0.49              |
| 25:RA:2275:C:O2   | 36:RQ:83:MET:HG3  | 2.11                     | 0.49              |
| 25:RA:2416:C:H5'' | 35:RP:64:LYS:HE3  | 1.93                     | 0.49              |
| 25:RA:2843:G:H1   | 25:RA:2874:C:H42  | 1.59                     | 0.49              |
| 26:RB:28:C:OP2    | 38:RS:33:LYS:HE3  | 2.13                     | 0.49              |
| 27:RD:2:ALA:CB    | 27:RD:20:ASP:HB3  | 2.42                     | 0.49              |
| 30:RG:6:ALA:H     | 50:R4:23:GLU:CG   | 2.25                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:114:ILE:HG21 | 30:RG:117:PHE:HB2  | 1.93                     | 0.49              |
| 31:RH:12:PRO:HD3   | 31:RH:48:GLY:O     | 2.13                     | 0.49              |
| 31:RH:24:VAL:HG21  | 31:RH:72:ILE:HG12  | 1.94                     | 0.49              |
| 31:RH:124:GLU:HB3  | 31:RH:132:ARG:CG   | 2.42                     | 0.49              |
| 35:RP:47:ASP:OD1   | 35:RP:49:ARG:NH1   | 2.46                     | 0.49              |
| 37:RR:41:ALA:C     | 37:RR:43:GLU:N     | 2.68                     | 0.49              |
| 38:RS:99:LYS:O     | 38:RS:101:LEU:N    | 2.45                     | 0.49              |
| 39:RT:94:ALA:O     | 39:RT:95:ARG:CB    | 2.61                     | 0.49              |
| 42:RW:48:ALA:O     | 42:RW:49:LYS:C     | 2.54                     | 0.49              |
| 50:R4:10:VAL:CG2   | 50:R4:11:PRO:HD2   | 2.43                     | 0.49              |
| 1:XA:1434:A:H2'    | 1:XA:1435:G:O4'    | 2.13                     | 0.49              |
| 4:XD:128:VAL:O     | 4:XD:130:GLY:N     | 2.45                     | 0.49              |
| 4:XD:163:GLU:O     | 4:XD:165:MET:N     | 2.46                     | 0.49              |
| 4:XD:206:PHE:HD2   | 4:XD:207:TYR:CE1   | 2.30                     | 0.49              |
| 5:XE:45:PHE:CD2    | 5:XE:47:LYS:HD2    | 2.47                     | 0.49              |
| 13:XM:3:ARG:HA     | 13:XM:9:ILE:HG12   | 1.94                     | 0.49              |
| 13:XM:73:GLU:O     | 13:XM:76:ALA:HB3   | 2.13                     | 0.49              |
| 15:XO:54:ARG:O     | 15:XO:55:GLY:C     | 2.55                     | 0.49              |
| 25:YA:749:C:H5'    | 25:YA:1271:G:H1'   | 1.95                     | 0.49              |
| 25:YA:1005:C:O2'   | 33:YN:28:THR:HG21  | 2.13                     | 0.49              |
| 34:YO:104:ARG:NH1  | 39:YT:36:GLU:CD    | 2.71                     | 0.49              |
| 35:YP:30:THR:O     | 35:YP:33:ARG:HB2   | 2.12                     | 0.49              |
| 35:YP:47:ASP:OD1   | 35:YP:49:ARG:NH1   | 2.46                     | 0.49              |
| 37:YR:96:ARG:NH2   | 37:YR:117:VAL:HG23 | 2.27                     | 0.49              |
| 40:YU:64:ARG:CG    | 40:YU:64:ARG:NH2   | 2.70                     | 0.49              |
| 44:YY:61:ILE:HG22  | 44:YY:62:GLU:N     | 2.28                     | 0.49              |
| 45:YZ:101:PRO:HA   | 45:YZ:123:ASP:HB3  | 1.94                     | 0.49              |
| 1:QA:430:A:H4'     | 4:QD:7:PRO:HG3     | 1.93                     | 0.49              |
| 1:QA:601:C:H2'     | 1:QA:602:A:C8      | 2.48                     | 0.49              |
| 1:QA:612:C:O2      | 1:QA:629:G:N2      | 2.46                     | 0.49              |
| 1:QA:1224:G:C6     | 1:QA:1322:C:H1'    | 2.47                     | 0.49              |
| 1:QA:1241:G:H2'    | 1:QA:1242:C:C6     | 2.48                     | 0.49              |
| 1:QA:1298:C:H4'    | 1:QA:1299:A:C8     | 2.47                     | 0.49              |
| 1:QA:1327:C:H2'    | 1:QA:1328:C:C6     | 2.48                     | 0.49              |
| 2:QB:16:HIS:HB3    | 2:QB:210:SER:HB2   | 1.95                     | 0.49              |
| 2:QB:42:ILE:HD11   | 2:QB:202:PRO:HB2   | 1.95                     | 0.49              |
| 2:QB:180:LEU:O     | 2:QB:181:PHE:HB2   | 2.12                     | 0.49              |
| 5:QE:51:VAL:CB     | 5:QE:52:PRO:HD3    | 2.38                     | 0.49              |
| 6:QF:97:PHE:CD2    | 18:QR:31:LEU:HD21  | 2.48                     | 0.49              |
| 9:QI:43:ALA:HA     | 9:QI:74:ILE:HD13   | 1.94                     | 0.49              |
| 9:QI:79:LEU:O      | 9:QI:83:ARG:HG2    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:QI:112:LYS:HD3  | 9:QI:113:LYS:O    | 2.13                     | 0.49              |
| 10:QJ:49:VAL:HG22 | 14:QN:41:ARG:CG   | 2.42                     | 0.49              |
| 11:QK:25:TYR:N    | 11:QK:25:TYR:CD1  | 2.80                     | 0.49              |
| 19:QS:26:GLY:O    | 19:QS:27:GLU:HB2  | 2.11                     | 0.49              |
| 25:RA:1262:A:N3   | 51:R5:10:LYS:HE3  | 2.28                     | 0.49              |
| 25:RA:1506:C:H3'  | 25:RA:1507:A:H5'' | 1.95                     | 0.49              |
| 25:RA:2572:A:N3   | 28:RE:144:ARG:NH2 | 2.61                     | 0.49              |
| 26:RB:111:U:H2'   | 26:RB:112:G:H8    | 1.78                     | 0.49              |
| 27:RD:30:GLU:CD   | 27:RD:63:ARG:HE   | 2.21                     | 0.49              |
| 28:RE:1:MET:H1    | 28:RE:1:MET:HE2   | 1.77                     | 0.49              |
| 28:RE:46:ALA:HB1  | 28:RE:80:GLU:HB2  | 1.94                     | 0.49              |
| 30:RG:143:GLU:HA  | 50:R4:28:LYS:HD3  | 1.95                     | 0.49              |
| 31:RH:137:ASP:CB  | 31:RH:140:LYS:HB2 | 2.43                     | 0.49              |
| 33:RN:73:THR:CG2  | 33:RN:82:LEU:HD11 | 2.43                     | 0.49              |
| 35:RP:101:VAL:CG1 | 35:RP:102:ARG:N   | 2.75                     | 0.49              |
| 39:RT:16:ARG:HD3  | 39:RT:19:LEU:CG   | 2.43                     | 0.49              |
| 39:RT:111:ARG:O   | 39:RT:112:ARG:CG  | 2.55                     | 0.49              |
| 42:RW:1:MET:HE2   | 42:RW:2:GLU:H     | 1.76                     | 0.49              |
| 44:RY:19:LYS:O    | 44:RY:19:LYS:CG   | 2.60                     | 0.49              |
| 44:RY:95:LYS:N    | 44:RY:95:LYS:CD   | 2.76                     | 0.49              |
| 47:R1:19:GLN:HA   | 47:R1:19:GLN:OE1  | 2.12                     | 0.49              |
| 47:R1:81:LYS:O    | 47:R1:82:LEU:O    | 2.30                     | 0.49              |
| 50:R4:68:ARG:HD3  | 50:R4:69:LYS:HG2  | 1.93                     | 0.49              |
| 51:R5:2:ALA:O     | 51:R5:3:LYS:CB    | 2.60                     | 0.49              |
| 51:R5:48:GLU:HA   | 51:R5:59:GLU:CG   | 2.43                     | 0.49              |
| 52:R6:7:ILE:C     | 52:R6:9:LEU:N     | 2.65                     | 0.49              |
| 52:R6:44:ARG:O    | 52:R6:45:LYS:CB   | 2.60                     | 0.49              |
| 1:XA:163:C:H2'    | 1:XA:164:U:C6     | 2.48                     | 0.49              |
| 1:XA:376:G:H5''   | 16:XP:5:ARG:HD2   | 1.95                     | 0.49              |
| 1:XA:701:C:H1'    | 1:XA:703:G:C4     | 2.48                     | 0.49              |
| 1:XA:1053:G:H2'   | 1:XA:1199:U:H5    | 1.78                     | 0.49              |
| 1:XA:1148:U:H2'   | 1:XA:1149:C:O4'   | 2.13                     | 0.49              |
| 1:XA:1342:C:H4'   | 9:XI:125:TYR:HB3  | 1.93                     | 0.49              |
| 2:XB:69:LEU:HB3   | 2:XB:162:ILE:HG22 | 1.95                     | 0.49              |
| 3:XC:76:VAL:HG21  | 3:XC:103:VAL:HG11 | 1.95                     | 0.49              |
| 4:XD:3:ARG:O      | 4:XD:4:TYR:C      | 2.55                     | 0.49              |
| 5:XE:62:ALA:C     | 5:XE:64:ARG:H     | 2.21                     | 0.49              |
| 9:XI:22:GLY:HA3   | 9:XI:60:ASP:OD2   | 2.13                     | 0.49              |
| 10:XJ:3:LYS:O     | 10:XJ:100:THR:HA  | 2.13                     | 0.49              |
| 10:XJ:16:LEU:HD13 | 10:XJ:16:LEU:C    | 2.38                     | 0.49              |
| 10:XJ:63:PHE:CD1  | 14:YN:58:LYS:HA   | 2.35                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:XK:13:GLN:HG3   | 11:XK:75:TYR:O    | 2.13                     | 0.49              |
| 12:XL:85:ILE:HD11  | 12:XL:98:TYR:CB   | 2.43                     | 0.49              |
| 14:XN:47:LEU:O     | 14:XN:48:ALA:C    | 2.56                     | 0.49              |
| 19:XS:11:VAL:O     | 19:XS:12:ASP:CB   | 2.61                     | 0.49              |
| 20:XT:37:SER:O     | 20:XT:41:ILE:HG12 | 2.12                     | 0.49              |
| 20:XT:60:GLU:HG3   | 20:XT:81:LYS:HE3  | 1.94                     | 0.49              |
| 20:XT:97:ALA:HB3   | 20:XT:99:LEU:CD1  | 2.43                     | 0.49              |
| 20:XT:98:PRO:C     | 20:XT:100:ILE:H   | 2.19                     | 0.49              |
| 25:YA:618(A):C:OP2 | 29:YF:103:LYS:HE2 | 2.12                     | 0.49              |
| 25:YA:1264:G:H5'   | 51:Y5:11:THR:HG21 | 1.94                     | 0.49              |
| 25:YA:1312:U:H4'   | 25:YA:1313:U:O5'  | 2.12                     | 0.49              |
| 25:YA:1543:A:O2'   | 25:YA:1544:C:P    | 2.71                     | 0.49              |
| 25:YA:2327:A:H2'   | 25:YA:2328:A:C8   | 2.48                     | 0.49              |
| 27:YD:69:ARG:C     | 27:YD:71:ASP:N    | 2.69                     | 0.49              |
| 27:YD:123:ALA:HB3  | 27:YD:131:LEU:HG  | 1.94                     | 0.49              |
| 28:YE:119:ARG:HD3  | 28:YE:160:TYR:CD2 | 2.47                     | 0.49              |
| 28:YE:179:GLU:HA   | 28:YE:179:GLU:OE1 | 2.10                     | 0.49              |
| 30:YG:3:LEU:HD21   | 50:Y4:25:TYR:CE1  | 2.48                     | 0.49              |
| 30:YG:115:ARG:HH11 | 30:YG:115:ARG:HG2 | 1.77                     | 0.49              |
| 31:YH:124:GLU:HB3  | 31:YH:132:ARG:CG  | 2.43                     | 0.49              |
| 32:YI:133:HIS:HB2  | 32:YI:134:PRO:HD2 | 1.94                     | 0.49              |
| 33:YN:4:TYR:OH     | 33:YN:7:LYS:NZ    | 2.46                     | 0.49              |
| 38:YS:11:LYS:HG2   | 38:YS:11:LYS:O    | 2.12                     | 0.49              |
| 41:YV:79:VAL:HG22  | 41:YV:79:VAL:O    | 2.12                     | 0.49              |
| 50:Y4:53:GLU:O     | 50:Y4:57:GLU:HG3  | 2.13                     | 0.49              |
| 1:QA:1194:U:H4'    | 5:QE:22:GLY:O     | 2.13                     | 0.49              |
| 1:QA:1346:A:N6     | 7:QG:10:ARG:HD2   | 2.28                     | 0.49              |
| 1:QA:1348:U:C4     | 1:QA:1374:A:H2    | 2.31                     | 0.49              |
| 1:QA:1485:U:H2'    | 1:QA:1486:G:H8    | 1.77                     | 0.49              |
| 2:QB:207:ALA:O     | 2:QB:209:ARG:N    | 2.45                     | 0.49              |
| 8:QH:122:ARG:O     | 8:QH:125:ARG:N    | 2.46                     | 0.49              |
| 10:QJ:49:VAL:CG1   | 10:QJ:50:ILE:N    | 2.76                     | 0.49              |
| 10:QJ:49:VAL:HG23  | 14:QN:34:TYR:OH   | 2.13                     | 0.49              |
| 11:QK:82:VAL:O     | 11:QK:108:ILE:HA  | 2.13                     | 0.49              |
| 13:QM:36:LYS:C     | 13:QM:36:LYS:CD   | 2.86                     | 0.49              |
| 17:QQ:63:ARG:HG2   | 17:QQ:64:PRO:N    | 2.28                     | 0.49              |
| 20:QT:84:LEU:C     | 20:QT:84:LEU:HD13 | 2.37                     | 0.49              |
| 25:RA:249:C:O2     | 54:R8:12:LYS:HE3  | 2.13                     | 0.49              |
| 26:RB:33:G:O5'     | 30:RG:2:PRO:HG3   | 2.12                     | 0.49              |
| 27:RD:233:HIS:CD2  | 27:RD:233:HIS:H   | 2.29                     | 0.49              |
| 28:RE:38:THR:O     | 28:RE:42:ASP:HB2  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:179:GLU:O   | 28:RE:180:ASN:HB2  | 2.13                     | 0.49              |
| 29:RF:45:ARG:NH1  | 29:RF:45:ARG:HG2   | 2.28                     | 0.49              |
| 29:RF:129:PHE:CD2 | 29:RF:163:VAL:HG21 | 2.48                     | 0.49              |
| 34:RO:107:ARG:NH1 | 39:RT:36:GLU:OE1   | 2.46                     | 0.49              |
| 35:RP:36:LYS:HB2  | 35:RP:40:SER:HB3   | 1.94                     | 0.49              |
| 36:RQ:31:ASP:O    | 36:RQ:32:TYR:CG    | 2.66                     | 0.49              |
| 37:RR:44:LEU:HD22 | 37:RR:48:VAL:CG2   | 2.42                     | 0.49              |
| 37:RR:52:ILE:CG2  | 37:RR:94:TYR:CD1   | 2.96                     | 0.49              |
| 41:RV:29:PRO:O    | 41:RV:61:VAL:HG22  | 2.12                     | 0.49              |
| 41:RV:79:VAL:HG22 | 41:RV:79:VAL:O     | 2.12                     | 0.49              |
| 43:RX:44:GLU:OE1  | 43:RX:50:LYS:HD2   | 2.13                     | 0.49              |
| 44:RY:101:LYS:O   | 44:RY:102:CYS:SG   | 2.66                     | 0.49              |
| 51:R5:45:VAL:O    | 51:R5:45:VAL:HG12  | 2.13                     | 0.49              |
| 51:R5:52:TYR:O    | 51:R5:53:ALA:CB    | 2.60                     | 0.49              |
| 52:R6:7:ILE:O     | 52:R6:9:LEU:N      | 2.46                     | 0.49              |
| 52:R6:8:LYS:O     | 52:R6:27:LYS:HA    | 2.13                     | 0.49              |
| 52:R6:27:LYS:NZ   | 52:R6:27:LYS:CB    | 2.73                     | 0.49              |
| 1:XA:246:A:N6     | 1:XA:281:G:H1'     | 2.28                     | 0.49              |
| 1:XA:1048:G:OP1   | 14:YN:3:ARG:HB3    | 2.12                     | 0.49              |
| 2:XB:7:VAL:CG2    | 2:XB:8:LYS:HD3     | 2.43                     | 0.49              |
| 2:XB:154:LEU:O    | 2:XB:155:LEU:HB2   | 2.13                     | 0.49              |
| 7:XG:23:VAL:O     | 7:XG:27:ILE:CD1    | 2.60                     | 0.49              |
| 7:XG:63:LYS:O     | 7:XG:63:LYS:HD2    | 2.13                     | 0.49              |
| 10:XJ:53:PRO:C    | 14:YN:41:ARG:NH2   | 2.71                     | 0.49              |
| 11:XK:41:THR:HG22 | 11:XK:42:TRP:N     | 2.28                     | 0.49              |
| 13:XM:11:ARG:HH21 | 30:YG:146:TYR:HD2  | 1.59                     | 0.49              |
| 13:XM:12:ASN:O    | 13:XM:13:LYS:HB2   | 2.13                     | 0.49              |
| 13:XM:16:ASP:HB3  | 13:XM:34:LEU:HD11  | 1.93                     | 0.49              |
| 13:XM:23:TYR:HB3  | 13:XM:67:GLU:CG    | 2.39                     | 0.49              |
| 20:XT:83:ARG:C    | 20:XT:86:ARG:HB3   | 2.38                     | 0.49              |
| 22:XV:75:C:H2'    | 22:XV:76:A:O4'     | 2.12                     | 0.49              |
| 25:YA:698:C:O2'   | 25:YA:734:A:N6     | 2.46                     | 0.49              |
| 25:YA:755:C:H2'   | 25:YA:756:C:H6     | 1.77                     | 0.49              |
| 25:YA:1219:G:OP2  | 40:YU:19:LYS:HD2   | 2.13                     | 0.49              |
| 25:YA:1266:G:O4'  | 42:YW:15:ARG:NH2   | 2.41                     | 0.49              |
| 27:YD:25:THR:O    | 27:YD:27:THR:HG22  | 2.12                     | 0.49              |
| 30:YG:143:GLU:HA  | 50:Y4:28:LYS:HD3   | 1.95                     | 0.49              |
| 31:YH:54:ARG:HD3  | 31:YH:65:HIS:ND1   | 2.27                     | 0.49              |
| 31:YH:153:LYS:CB  | 31:YH:154:PRO:CD   | 2.69                     | 0.49              |
| 32:YI:75:LEU:HB3  | 32:YI:105:HIS:CD2  | 2.48                     | 0.49              |
| 35:YP:31:ALA:C    | 35:YP:32:THR:CG2   | 2.85                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:YP:101:VAL:CG1 | 35:YP:102:ARG:N    | 2.75                     | 0.49              |
| 36:YQ:23:GLY:O    | 36:YQ:24:GLY:O     | 2.30                     | 0.49              |
| 36:YQ:86:GLY:O    | 36:YQ:88:GLY:N     | 2.46                     | 0.49              |
| 37:YR:41:ALA:C    | 37:YR:43:GLU:H     | 2.20                     | 0.49              |
| 37:YR:41:ALA:C    | 37:YR:43:GLU:N     | 2.68                     | 0.49              |
| 38:YS:48:LEU:N    | 38:YS:48:LEU:CD1   | 2.76                     | 0.49              |
| 42:YW:88:ARG:HB3  | 42:YW:92:ARG:CB    | 2.42                     | 0.49              |
| 52:Y6:9:LEU:HD13  | 52:Y6:26:ASN:HD22  | 1.76                     | 0.49              |
| 52:Y6:37:ARG:HE   | 52:Y6:37:ARG:HA    | 1.77                     | 0.49              |
| 54:Y8:15:LYS:HD3  | 54:Y8:15:LYS:C     | 2.37                     | 0.49              |
| 54:Y8:35:GLN:HA   | 54:Y8:35:GLN:OE1   | 2.12                     | 0.49              |
| 54:Y8:52:LYS:H    | 54:Y8:53:PRO:HD2   | 1.66                     | 0.49              |
| 1:QA:193:C:H2'    | 1:QA:194:C:C6      | 2.48                     | 0.48              |
| 1:QA:914:A:H2'    | 1:QA:915:A:H8      | 1.79                     | 0.48              |
| 1:QA:1119:C:H2'   | 1:QA:1120:G:C8     | 2.48                     | 0.48              |
| 1:QA:1129:C:H4'   | 1:QA:1130:A:H5'    | 1.95                     | 0.48              |
| 2:QB:68:ILE:O     | 2:QB:91:PRO:HD2    | 2.13                     | 0.48              |
| 2:QB:178:ARG:HD2  | 8:QH:71:GLY:C      | 2.38                     | 0.48              |
| 2:QB:193:ASP:OD2  | 2:QB:196:LEU:CG    | 2.57                     | 0.48              |
| 3:QC:188:LEU:N    | 3:QC:188:LEU:CD2   | 2.76                     | 0.48              |
| 4:QD:68:TYR:O     | 4:QD:69:GLY:C      | 2.55                     | 0.48              |
| 5:QE:78:HIS:CE1   | 5:QE:142:LEU:HD23  | 2.48                     | 0.48              |
| 6:QF:72:VAL:HG13  | 6:QF:73:ASN:N      | 2.27                     | 0.48              |
| 8:QH:61:VAL:HG12  | 8:QH:63:LEU:HD13   | 1.95                     | 0.48              |
| 10:QJ:94:VAL:CG1  | 10:QJ:95:GLU:N     | 2.76                     | 0.48              |
| 11:QK:106:LYS:O   | 11:QK:107:SER:HB3  | 2.11                     | 0.48              |
| 25:RA:608:A:H2'   | 25:RA:609:A:C8     | 2.48                     | 0.48              |
| 25:RA:1022:G:H22  | 25:RA:1142(A):A:H2 | 1.61                     | 0.48              |
| 25:RA:2562:U:H1'  | 34:RO:23:ARG:NH1   | 2.29                     | 0.48              |
| 26:RB:12:C:H2'    | 46:R0:73:GLY:HA3   | 1.95                     | 0.48              |
| 30:RG:77:ILE:O    | 30:RG:81:LYS:O     | 2.31                     | 0.48              |
| 30:RG:115:ARG:HG2 | 30:RG:115:ARG:NH1  | 2.27                     | 0.48              |
| 31:RH:123:PHE:O   | 31:RH:125:VAL:HG23 | 2.13                     | 0.48              |
| 35:RP:30:THR:O    | 35:RP:33:ARG:HB2   | 2.12                     | 0.48              |
| 38:RS:48:LEU:N    | 38:RS:48:LEU:CD1   | 2.76                     | 0.48              |
| 41:RV:18:LEU:HB3  | 41:RV:96:ILE:CG1   | 2.43                     | 0.48              |
| 43:RX:11:PRO:HB3  | 43:RX:92:LEU:CD2   | 2.43                     | 0.48              |
| 44:RY:6:HIS:O     | 44:RY:7:VAL:CG1    | 2.59                     | 0.48              |
| 45:RZ:45:ASP:O    | 45:RZ:49:ARG:HG2   | 2.13                     | 0.48              |
| 48:R2:69:ARG:HH11 | 48:R2:69:ARG:HB3   | 1.78                     | 0.48              |
| 50:R4:47:GLN:O    | 50:R4:48:ARG:CB    | 2.61                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:R5:3:LYS:O      | 51:R5:4:HIS:C     | 2.56                     | 0.48              |
| 54:R8:58:ILE:O     | 54:R8:61:LEU:HD12 | 2.13                     | 0.48              |
| 1:XA:34:C:H2'      | 1:XA:35:G:C8      | 2.48                     | 0.48              |
| 1:XA:573:A:N3      | 1:XA:883:C:O2'    | 2.39                     | 0.48              |
| 1:XA:1306:A:N6     | 1:XA:1331:G:H1'   | 2.28                     | 0.48              |
| 2:XB:181:PHE:O     | 2:XB:183:PRO:HD3  | 2.12                     | 0.48              |
| 5:XE:12:LEU:HD23   | 5:XE:13:ILE:H     | 1.77                     | 0.48              |
| 9:XI:79:LEU:O      | 9:XI:79:LEU:HD13  | 2.12                     | 0.48              |
| 16:XP:57:ARG:HH11  | 16:XP:57:ARG:HG3  | 1.78                     | 0.48              |
| 21:XU:9:ARG:HH11   | 21:XU:9:ARG:HG2   | 1.78                     | 0.48              |
| 25:YA:507:A:C5'    | 25:YA:508:G:H5'   | 2.42                     | 0.48              |
| 25:YA:2154:G:H2'   | 25:YA:2155:G:H8   | 1.77                     | 0.48              |
| 26:YB:48:A:H4'     | 38:YS:95:HIS:HD2  | 1.77                     | 0.48              |
| 30:YG:77:ILE:O     | 30:YG:81:LYS:O    | 2.31                     | 0.48              |
| 35:YP:6:LEU:O      | 35:YP:7:ARG:O     | 2.31                     | 0.48              |
| 35:YP:52:GLU:OE2   | 35:YP:57:THR:HA   | 2.13                     | 0.48              |
| 35:YP:144:GLU:O    | 35:YP:144:GLU:OE1 | 2.31                     | 0.48              |
| 36:YQ:34:LEU:HD23  | 36:YQ:104:PHE:HD1 | 1.77                     | 0.48              |
| 37:YR:33:ARG:NH2   | 51:Y5:55:ARG:CG   | 2.66                     | 0.48              |
| 38:YS:55:ALA:O     | 38:YS:56:LEU:HB3  | 2.14                     | 0.48              |
| 48:Y2:16:LEU:O     | 48:Y2:17:SER:CB   | 2.56                     | 0.48              |
| 51:Y5:49:CYS:SG    | 51:Y5:58:LEU:HB2  | 2.53                     | 0.48              |
| 54:Y8:33:ASN:O     | 54:Y8:35:GLN:N    | 2.46                     | 0.48              |
| 1:QA:6:G:H4'       | 1:QA:298:A:H4'    | 1.95                     | 0.48              |
| 1:QA:1405:G:O2'    | 1:QA:1518:A:O3'   | 2.31                     | 0.48              |
| 2:QB:7:VAL:CG2     | 2:QB:8:LYS:HD3    | 2.43                     | 0.48              |
| 2:QB:39:ILE:O      | 2:QB:41:ILE:HD12  | 2.12                     | 0.48              |
| 20:QT:26:ASN:CB    | 20:QT:71:THR:HG23 | 2.43                     | 0.48              |
| 25:RA:242:G:H5''   | 54:R8:3:LYS:HE3   | 1.95                     | 0.48              |
| 25:RA:593:G:O2'    | 54:R8:61:LEU:HD13 | 2.13                     | 0.48              |
| 25:RA:704:G:C2'    | 25:RA:726:G:H22   | 2.25                     | 0.48              |
| 25:RA:2064:C:H2'   | 25:RA:2065:C:C6   | 2.48                     | 0.48              |
| 29:RF:155:LEU:HD23 | 29:RF:186:ILE:HA  | 1.95                     | 0.48              |
| 30:RG:36:LYS:HA    | 30:RG:95:ARG:HG2  | 1.95                     | 0.48              |
| 31:RH:42:ARG:O     | 31:RH:52:VAL:HA   | 2.13                     | 0.48              |
| 31:RH:119:GLU:CD   | 31:RH:120:GLY:H   | 2.22                     | 0.48              |
| 32:RI:93:THR:O     | 32:RI:97:ILE:HG12 | 2.11                     | 0.48              |
| 32:RI:116:LEU:O    | 32:RI:118:LYS:N   | 2.45                     | 0.48              |
| 34:RO:104:ARG:NH1  | 39:RT:36:GLU:CD   | 2.71                     | 0.48              |
| 37:RR:42:LYS:HA    | 37:RR:45:ARG:HD2  | 1.95                     | 0.48              |
| 38:RS:11:LYS:O     | 38:RS:11:LYS:HG2  | 2.12                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:RV:22:VAL:HG12 | 41:RV:23:GLU:H     | 1.76                     | 0.48              |
| 41:RV:35:LEU:HD22 | 41:RV:57:VAL:O     | 2.13                     | 0.48              |
| 42:RW:36:LEU:CD1  | 42:RW:47:VAL:HG12  | 2.43                     | 0.48              |
| 42:RW:51:LEU:HD23 | 42:RW:105:VAL:HG11 | 1.95                     | 0.48              |
| 43:RX:35:THR:O    | 43:RX:37:THR:N     | 2.46                     | 0.48              |
| 47:R1:93:GLU:O    | 47:R1:97:LEU:HD11  | 2.12                     | 0.48              |
| 48:R2:15:LYS:H    | 48:R2:67:LYS:HZ3   | 1.61                     | 0.48              |
| 1:XA:191:G:O2'    | 20:XT:101:GLY:O    | 2.31                     | 0.48              |
| 1:XA:328:C:H4'    | 1:XA:329:A:C5'     | 2.41                     | 0.48              |
| 1:XA:377:G:OP1    | 16:XP:5:ARG:NH1    | 2.45                     | 0.48              |
| 1:XA:545:C:OP2    | 4:XD:62:GLN:NE2    | 2.45                     | 0.48              |
| 1:XA:824:C:H2'    | 1:XA:825:G:C8      | 2.48                     | 0.48              |
| 1:XA:953:G:H2'    | 1:XA:954:G:O4'     | 2.12                     | 0.48              |
| 2:XB:16:HIS:HB3   | 2:XB:210:SER:HB2   | 1.95                     | 0.48              |
| 2:XB:39:ILE:O     | 2:XB:41:ILE:HD12   | 2.13                     | 0.48              |
| 2:XB:134:GLU:HB3  | 2:XB:138:LEU:HD12  | 1.93                     | 0.48              |
| 2:XB:180:LEU:O    | 2:XB:181:PHE:HB2   | 2.13                     | 0.48              |
| 2:XB:206:ASP:HA   | 2:XB:211:ILE:HD11  | 1.94                     | 0.48              |
| 3:XC:14:ILE:C     | 3:XC:16:ARG:H      | 2.21                     | 0.48              |
| 4:XD:180:GLY:O    | 4:XD:181:MET:C     | 2.54                     | 0.48              |
| 7:XG:107:ALA:CB   | 7:XG:134:ALA:HB2   | 2.44                     | 0.48              |
| 8:XH:82:HIS:CD2   | 8:XH:82:HIS:C      | 2.91                     | 0.48              |
| 9:XI:18:PHE:O     | 9:XI:61:ALA:HA     | 2.13                     | 0.48              |
| 9:XI:79:LEU:O     | 9:XI:83:ARG:HG2    | 2.13                     | 0.48              |
| 13:XM:65:LYS:HZ3  | 13:XM:69:GLU:HG2   | 1.77                     | 0.48              |
| 16:XP:43:LYS:HE2  | 16:XP:48:TRP:CZ3   | 2.48                     | 0.48              |
| 17:XQ:67:LYS:HA   | 17:XQ:70:ARG:HH12  | 1.76                     | 0.48              |
| 25:YA:25:U:H5''   | 42:YW:80:PRO:HD3   | 1.94                     | 0.48              |
| 25:YA:49:A:N7     | 25:YA:120:U:H5     | 2.11                     | 0.48              |
| 25:YA:489:G:N2    | 25:YA:1321:A:OP1   | 2.46                     | 0.48              |
| 25:YA:686:G:H8    | 53:Y7:6:GLN:O      | 1.96                     | 0.48              |
| 25:YA:1031:G:O2'  | 55:Y9:7:VAL:O      | 2.27                     | 0.48              |
| 25:YA:1432:C:H2'  | 25:YA:1433:U:O4'   | 2.13                     | 0.48              |
| 25:YA:2442:C:H2'  | 25:YA:2443:C:H6    | 1.77                     | 0.48              |
| 26:YB:50:G:OP1    | 38:YS:63:THR:HG23  | 2.12                     | 0.48              |
| 30:YG:92:VAL:O    | 30:YG:92:VAL:HG13  | 2.12                     | 0.48              |
| 30:YG:113:ARG:HD2 | 50:Y4:33:VAL:CG1   | 2.43                     | 0.48              |
| 31:YH:13:LYS:HE2  | 31:YH:13:LYS:CA    | 2.40                     | 0.48              |
| 31:YH:137:ASP:CB  | 31:YH:140:LYS:HB2  | 2.43                     | 0.48              |
| 36:YQ:90:VAL:C    | 36:YQ:92:GLY:N     | 2.71                     | 0.48              |
| 37:YR:71:GLN:HE21 | 37:YR:71:GLN:HA    | 1.77                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:YV:7:THR:HG23  | 41:YV:22:VAL:HG11  | 1.94                     | 0.48              |
| 41:YV:35:LEU:HD22 | 41:YV:57:VAL:O     | 2.13                     | 0.48              |
| 41:YV:76:LYS:HG3  | 41:YV:81:TYR:CD1   | 2.48                     | 0.48              |
| 44:YY:97:ARG:HG2  | 44:YY:97:ARG:NH1   | 2.28                     | 0.48              |
| 47:Y1:56:GLN:NE2  | 47:Y1:56:GLN:H     | 2.10                     | 0.48              |
| 51:Y5:48:GLU:HA   | 51:Y5:59:GLU:HG2   | 1.94                     | 0.48              |
| 53:Y7:48:LYS:CG   | 53:Y7:49:ARG:H     | 2.23                     | 0.48              |
| 2:QB:5:ILE:HG21   | 2:QB:224:GLN:HG2   | 1.95                     | 0.48              |
| 4:QD:196:LEU:HB3  | 4:QD:197:PRO:HD2   | 1.95                     | 0.48              |
| 5:QE:100:VAL:O    | 5:QE:107:ARG:NH2   | 2.47                     | 0.48              |
| 11:QK:19:ALA:CB   | 11:QK:32:ILE:HG22  | 2.42                     | 0.48              |
| 11:QK:53:SER:C    | 11:QK:55:LYS:H     | 2.20                     | 0.48              |
| 12:QL:38:THR:CG2  | 12:QL:57:LYS:HB3   | 2.44                     | 0.48              |
| 14:QN:23:ARG:HD3  | 14:QN:28:GLY:O     | 2.13                     | 0.48              |
| 19:QS:27:GLU:O    | 19:QS:28:LYS:CG    | 2.53                     | 0.48              |
| 25:RA:128:C:H2'   | 25:RA:129:C:H6     | 1.78                     | 0.48              |
| 25:RA:2630:G:O4'  | 25:RA:2894:G:H1'   | 2.13                     | 0.48              |
| 27:RD:10:THR:O    | 27:RD:11:PRO:C     | 2.56                     | 0.48              |
| 30:RG:115:ARG:HG2 | 30:RG:115:ARG:HH11 | 1.77                     | 0.48              |
| 31:RH:109:PHE:C   | 31:RH:111:HIS:H    | 2.21                     | 0.48              |
| 35:RP:35:HIS:O    | 35:RP:36:LYS:O     | 2.31                     | 0.48              |
| 35:RP:52:GLU:OE2  | 35:RP:57:THR:HA    | 2.13                     | 0.48              |
| 37:RR:41:ALA:C    | 37:RR:43:GLU:H     | 2.21                     | 0.48              |
| 38:RS:33:LYS:HB3  | 38:RS:34:HIS:CD2   | 2.48                     | 0.48              |
| 39:RT:135:ALA:C   | 39:RT:137:LYS:N    | 2.71                     | 0.48              |
| 45:RZ:54:HIS:NE2  | 45:RZ:101:PRO:HG3  | 2.28                     | 0.48              |
| 48:R2:69:ARG:CB   | 48:R2:69:ARG:HH11  | 2.24                     | 0.48              |
| 50:R4:42:PHE:CD1  | 50:R4:42:PHE:C     | 2.90                     | 0.48              |
| 50:R4:48:ARG:C    | 50:R4:49:PHE:HD1   | 2.22                     | 0.48              |
| 1:XA:1152:A:H2'   | 1:XA:1153:C:C6     | 2.48                     | 0.48              |
| 1:XA:1399:C:C2    | 1:XA:1502:A:N6     | 2.81                     | 0.48              |
| 5:XE:60:TYR:CE1   | 5:XE:64:ARG:NH2    | 2.77                     | 0.48              |
| 5:XE:83:GLU:HG2   | 5:XE:88:LYS:CG     | 2.42                     | 0.48              |
| 6:XF:51:PRO:HA    | 6:XF:55:ASP:O      | 2.13                     | 0.48              |
| 7:XG:80:VAL:HG12  | 7:XG:81:GLY:N      | 2.28                     | 0.48              |
| 8:XH:45:ILE:O     | 8:XH:45:ILE:HG13   | 2.13                     | 0.48              |
| 10:XJ:33:GLN:HB2  | 10:XJ:75:ILE:CD1   | 2.43                     | 0.48              |
| 10:XJ:49:VAL:CG1  | 10:XJ:50:ILE:N     | 2.75                     | 0.48              |
| 16:XP:39:TYR:CE2  | 16:XP:41:PRO:HD3   | 2.47                     | 0.48              |
| 25:YA:1681:G:H8   | 25:YA:1681:G:OP2   | 1.96                     | 0.48              |
| 25:YA:2795:G:H3'  | 25:YA:2797:U:C5'   | 2.43                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:YB:42:C:C6     | 30:YG:69:ALA:HB2   | 2.48                     | 0.48              |
| 27:YD:44:ASN:H    | 27:YD:44:ASN:ND2   | 1.97                     | 0.48              |
| 30:YG:115:ARG:NH1 | 30:YG:115:ARG:HG2  | 2.26                     | 0.48              |
| 31:YH:12:PRO:HD3  | 31:YH:48:GLY:O     | 2.13                     | 0.48              |
| 32:YI:11:ASN:O    | 32:YI:12:LEU:HB2   | 2.14                     | 0.48              |
| 32:YI:30:LEU:HB3  | 32:YI:36:ALA:HB3   | 1.94                     | 0.48              |
| 35:YP:71:VAL:HG13 | 35:YP:72:PRO:CD    | 2.43                     | 0.48              |
| 38:YS:33:LYS:HB3  | 38:YS:34:HIS:CD2   | 2.48                     | 0.48              |
| 44:YY:81:LYS:HD3  | 44:YY:97:ARG:HD3   | 1.94                     | 0.48              |
| 45:YZ:112:ARG:O   | 45:YZ:114:GLY:N    | 2.46                     | 0.48              |
| 47:Y1:73:LEU:C    | 47:Y1:75:GLU:N     | 2.70                     | 0.48              |
| 52:Y6:7:ILE:O     | 52:Y6:9:LEU:N      | 2.46                     | 0.48              |
| 1:QA:857:C:H2'    | 1:QA:858:G:O4'     | 2.14                     | 0.48              |
| 1:QA:1129:C:O2'   | 1:QA:1131:G:N7     | 2.46                     | 0.48              |
| 4:QD:118:ARG:NH2  | 4:QD:136:PRO:HB2   | 2.28                     | 0.48              |
| 9:QI:18:PHE:HB2   | 9:QI:62:TYR:HB3    | 1.96                     | 0.48              |
| 9:QI:118:LYS:NZ   | 9:QI:118:LYS:CB    | 2.75                     | 0.48              |
| 13:QM:69:GLU:O    | 13:QM:70:LEU:C     | 2.56                     | 0.48              |
| 19:QS:36:ARG:HB3  | 19:QS:36:ARG:NH1   | 2.28                     | 0.48              |
| 25:RA:518:G:H4'   | 42:RW:18:ARG:NH1   | 2.17                     | 0.48              |
| 25:RA:2271:G:H2'  | 25:RA:2272:U:C6    | 2.48                     | 0.48              |
| 25:RA:2325:G:H8   | 25:RA:2325:G:O5'   | 1.95                     | 0.48              |
| 25:RA:2630:G:N3   | 25:RA:2894:G:N2    | 2.61                     | 0.48              |
| 26:RB:13:A:O2'    | 26:RB:14:U:H3'     | 2.13                     | 0.48              |
| 26:RB:24:G:H5''   | 26:RB:25:A:OP1     | 2.14                     | 0.48              |
| 28:RE:78:LEU:CD2  | 28:RE:79:ARG:HD2   | 2.44                     | 0.48              |
| 30:RG:125:PHE:HB3 | 30:RG:166:ASP:HB2  | 1.95                     | 0.48              |
| 31:RH:104:GLU:HG3 | 31:RH:114:VAL:HG22 | 1.96                     | 0.48              |
| 39:RT:105:LEU:C   | 39:RT:107:ASP:OD1  | 2.56                     | 0.48              |
| 39:RT:132:LYS:O   | 39:RT:136:GLN:HG3  | 2.14                     | 0.48              |
| 41:RV:6:LYS:HD3   | 41:RV:11:GLN:HG2   | 1.96                     | 0.48              |
| 46:R0:40:GLN:OE1  | 46:R0:45:PHE:N     | 2.46                     | 0.48              |
| 51:R5:56:LYS:HD2  | 51:R5:56:LYS:N     | 2.13                     | 0.48              |
| 52:R6:14:THR:OG1  | 52:R6:19:ARG:NE    | 2.40                     | 0.48              |
| 54:R8:35:GLN:HA   | 54:R8:35:GLN:OE1   | 2.12                     | 0.48              |
| 54:R8:56:GLU:O    | 54:R8:58:ILE:N     | 2.47                     | 0.48              |
| 1:XA:21:G:H2'     | 1:XA:22:G:C8       | 2.48                     | 0.48              |
| 1:XA:757:U:H2'    | 1:XA:758:G:O4'     | 2.14                     | 0.48              |
| 1:XA:1059:C:H2'   | 1:XA:1060:C:H6     | 1.79                     | 0.48              |
| 1:XA:1297:C:H4'   | 1:XA:1298:C:H5'    | 1.95                     | 0.48              |
| 2:XB:16:HIS:HD2   | 2:XB:210:SER:HA    | 1.77                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:XB:42:ILE:HD11 | 2:XB:202:PRO:HB2  | 1.95                     | 0.48              |
| 4:XD:3:ARG:O     | 4:XD:5:ILE:HG13   | 2.14                     | 0.48              |
| 4:XD:121:VAL:O   | 4:XD:134:ASP:HA   | 2.13                     | 0.48              |
| 9:XI:112:LYS:HD3 | 9:XI:113:LYS:O    | 2.13                     | 0.48              |
| 10:XJ:56:HIS:O   | 10:XJ:58:ASP:O    | 2.30                     | 0.48              |
| 10:XJ:98:ILE:H   | 10:XJ:98:ILE:CD1  | 2.24                     | 0.48              |
| 11:XK:96:ARG:O   | 11:XK:97:ALA:C    | 2.54                     | 0.48              |
| 12:XL:27:LEU:C   | 12:XL:29:GLY:H    | 2.20                     | 0.48              |
| 12:XL:38:THR:CG2 | 12:XL:57:LYS:HB3  | 2.44                     | 0.48              |
| 16:XP:69:THR:O   | 16:XP:73:LEU:HG   | 2.14                     | 0.48              |
| 25:YA:153:C:OP2  | 47:Y1:88:LYS:HE2  | 2.13                     | 0.48              |
| 25:YA:2115:G:N2  | 25:YA:2165:G:N7   | 2.56                     | 0.48              |
| 27:YD:45:ASN:CG  | 27:YD:46:GLN:N    | 2.68                     | 0.48              |
| 27:YD:48:ARG:HG3 | 27:YD:48:ARG:HH11 | 1.78                     | 0.48              |
| 31:YH:23:ARG:HD2 | 31:YH:34:GLU:OE2  | 2.12                     | 0.48              |
| 31:YH:42:ARG:O   | 31:YH:52:VAL:HA   | 2.13                     | 0.48              |
| 31:YH:109:PHE:C  | 31:YH:111:HIS:H   | 2.22                     | 0.48              |
| 33:YN:30:ILE:O   | 33:YN:34:LEU:HD23 | 2.13                     | 0.48              |
| 35:YP:6:LEU:N    | 35:YP:6:LEU:CD2   | 2.75                     | 0.48              |
| 37:YR:52:ILE:CG2 | 37:YR:94:TYR:CD1  | 2.95                     | 0.48              |
| 40:YU:52:ARG:NH1 | 40:YU:52:ARG:CG   | 2.76                     | 0.48              |
| 40:YU:79:PHE:C   | 40:YU:79:PHE:HD2  | 2.18                     | 0.48              |
| 40:YU:91:ASP:O   | 40:YU:95:LEU:N    | 2.42                     | 0.48              |
| 41:YV:18:LEU:HB3 | 41:YV:96:ILE:CG1  | 2.43                     | 0.48              |
| 44:YY:11:ASP:HB2 | 44:YY:27:VAL:HG11 | 1.94                     | 0.48              |
| 44:YY:35:TYR:CD1 | 44:YY:69:ALA:HB3  | 2.48                     | 0.48              |
| 44:YY:77:PRO:O   | 44:YY:78:ALA:HB2  | 2.11                     | 0.48              |
| 53:Y7:12:ARG:HG3 | 53:Y7:12:ARG:HH11 | 1.78                     | 0.48              |
| 1:QA:475:G:H2'   | 1:QA:476:G:H8     | 1.79                     | 0.48              |
| 1:QA:624:C:H2'   | 1:QA:625:G:H8     | 1.78                     | 0.48              |
| 2:QB:214:ILE:O   | 2:QB:218:ALA:HB2  | 2.14                     | 0.48              |
| 4:QD:25:ARG:C    | 4:QD:27:TYR:H     | 2.21                     | 0.48              |
| 4:QD:100:ARG:CZ  | 4:QD:137:SER:HA   | 2.43                     | 0.48              |
| 4:QD:121:VAL:O   | 4:QD:134:ASP:HA   | 2.14                     | 0.48              |
| 7:QG:78:ARG:HG3  | 7:QG:78:ARG:HH11  | 1.79                     | 0.48              |
| 7:QG:80:VAL:HG12 | 7:QG:81:GLY:N     | 2.28                     | 0.48              |
| 8:QH:14:ARG:O    | 8:QH:14:ARG:HG2   | 2.12                     | 0.48              |
| 9:QI:113:LYS:H   | 9:QI:119:ALA:HA   | 1.77                     | 0.48              |
| 10:QJ:3:LYS:O    | 10:QJ:100:THR:HA  | 2.13                     | 0.48              |
| 13:QM:3:ARG:HA   | 13:QM:9:ILE:HG12  | 1.94                     | 0.48              |
| 15:QO:50:HIS:O   | 15:QO:53:HIS:N    | 2.47                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 17:QQ:67:LYS:HA  | 17:QQ:70:ARG:HH12  | 1.77                     | 0.48              |
| 22:QV:4:G:O2'    | 22:QV:5:G:H8       | 1.96                     | 0.48              |
| 25:RA:395:U:H2'  | 25:RA:396:G:N7     | 2.28                     | 0.48              |
| 25:RA:706:A:H2'  | 25:RA:707:G:O4'    | 2.13                     | 0.48              |
| 25:RA:845:G:H8   | 25:RA:845:G:OP2    | 1.96                     | 0.48              |
| 25:RA:1818:U:H2' | 27:RD:157:ARG:HG3  | 1.96                     | 0.48              |
| 25:RA:2517:C:N3  | 25:RA:2542:A:N6    | 2.60                     | 0.48              |
| 25:RA:2892:A:H2' | 25:RA:2893:G:O4'   | 2.12                     | 0.48              |
| 27:RD:35:LYS:HD2 | 27:RD:104:TYR:CE1  | 2.49                     | 0.48              |
| 29:RF:128:ALA:O  | 29:RF:129:PHE:HB2  | 2.13                     | 0.48              |
| 29:RF:198:ALA:O  | 29:RF:201:VAL:HG12 | 2.13                     | 0.48              |
| 33:RN:10:GLU:HA  | 33:RN:11:PRO:HD3   | 1.73                     | 0.48              |
| 36:RQ:87:LYS:O   | 36:RQ:89:ASN:N     | 2.43                     | 0.48              |
| 44:RY:44:ILE:O   | 44:RY:62:GLU:O     | 2.32                     | 0.48              |
| 52:R6:27:LYS:O   | 52:R6:28:ARG:HG2   | 2.13                     | 0.48              |
| 53:R7:12:ARG:HG3 | 53:R7:12:ARG:HH11  | 1.78                     | 0.48              |
| 1:XA:1043:C:H2'  | 1:XA:1044:A:H8     | 1.77                     | 0.48              |
| 1:XA:1241:G:H2'  | 1:XA:1242:C:C6     | 2.49                     | 0.48              |
| 2:XB:5:ILE:HG21  | 2:XB:224:GLN:HG2   | 1.96                     | 0.48              |
| 2:XB:97:TRP:HZ2  | 2:XB:102:LEU:HD13  | 1.78                     | 0.48              |
| 3:XC:173:VAL:N   | 3:XC:174:PRO:HD3   | 2.27                     | 0.48              |
| 4:XD:9:CYS:SG    | 4:XD:22:LYS:CE     | 3.01                     | 0.48              |
| 4:XD:33:MET:CE   | 4:XD:37:PRO:HA     | 2.42                     | 0.48              |
| 5:XE:20:GLN:O    | 5:XE:21:ALA:C      | 2.57                     | 0.48              |
| 9:XI:118:LYS:NZ  | 9:XI:118:LYS:CB    | 2.75                     | 0.48              |
| 10:XJ:94:VAL:CG1 | 10:XJ:95:GLU:N     | 2.76                     | 0.48              |
| 11:XK:34:ASP:HB2 | 11:XK:35:PRO:HD2   | 1.95                     | 0.48              |
| 13:XM:50:GLU:O   | 13:XM:54:VAL:HG23  | 2.13                     | 0.48              |
| 19:XS:43:GLU:OE2 | 19:XS:43:GLU:N     | 2.45                     | 0.48              |
| 20:XT:37:SER:HB3 | 20:XT:84:LEU:CD2   | 2.43                     | 0.48              |
| 20:XT:53:LEU:HA  | 20:XT:56:MET:CB    | 2.43                     | 0.48              |
| 22:XV:4:G:O2'    | 22:XV:5:G:H8       | 1.96                     | 0.48              |
| 25:YA:189:G:H2'  | 25:YA:205:G:N2     | 2.29                     | 0.48              |
| 25:YA:676:A:H2   | 25:YA:802:A:H61    | 1.58                     | 0.48              |
| 25:YA:780:G:H8   | 25:YA:780:G:O5'    | 1.96                     | 0.48              |
| 25:YA:826:U:H2'  | 25:YA:828:U:O4'    | 2.12                     | 0.48              |
| 25:YA:1059:G:H3' | 25:YA:1060:U:H5''  | 1.94                     | 0.48              |
| 25:YA:2126:A:H4' | 25:YA:2127:G:O5'   | 2.13                     | 0.48              |
| 25:YA:2455:G:H2' | 25:YA:2456:C:C6    | 2.48                     | 0.48              |
| 27:YD:10:THR:O   | 27:YD:11:PRO:C     | 2.56                     | 0.48              |
| 28:YE:69:LYS:C   | 28:YE:71:GLY:N     | 2.71                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:174:ASP:O    | 28:YE:182:LEU:HD12 | 2.14                     | 0.48              |
| 29:YF:107:LYS:O    | 29:YF:110:LEU:N    | 2.47                     | 0.48              |
| 29:YF:128:ALA:O    | 29:YF:129:PHE:HB2  | 2.13                     | 0.48              |
| 29:YF:155:LEU:HD23 | 29:YF:186:ILE:HA   | 1.95                     | 0.48              |
| 29:YF:198:ALA:O    | 29:YF:201:VAL:HG12 | 2.13                     | 0.48              |
| 31:YH:82:GLY:O     | 31:YH:83:TYR:O     | 2.31                     | 0.48              |
| 32:YI:97:ILE:HD12  | 32:YI:140:LEU:HD11 | 1.96                     | 0.48              |
| 33:YN:87:LEU:C     | 33:YN:87:LEU:CD2   | 2.87                     | 0.48              |
| 39:YT:16:ARG:HD3   | 39:YT:19:LEU:CG    | 2.43                     | 0.48              |
| 47:Y1:8:SER:OG     | 47:Y1:10:LYS:HG3   | 2.13                     | 0.48              |
| 47:Y1:60:PHE:HE2   | 47:Y1:91:LYS:HZ1   | 1.59                     | 0.48              |
| 50:Y4:10:VAL:CG2   | 50:Y4:11:PRO:HD2   | 2.43                     | 0.48              |
| 51:Y5:52:TYR:O     | 51:Y5:53:ALA:CB    | 2.61                     | 0.48              |
| 52:Y6:27:LYS:O     | 52:Y6:28:ARG:HG2   | 2.13                     | 0.48              |
| 1:QA:191(D):U:H2'  | 1:QA:191(E):G:H8   | 1.77                     | 0.48              |
| 2:QB:15:VAL:H      | 2:QB:16:HIS:CE1    | 2.30                     | 0.48              |
| 2:QB:16:HIS:HD2    | 2:QB:210:SER:HA    | 1.77                     | 0.48              |
| 2:QB:154:LEU:O     | 2:QB:155:LEU:HB2   | 2.13                     | 0.48              |
| 2:QB:200:ILE:H     | 2:QB:200:ILE:HD12  | 1.79                     | 0.48              |
| 2:QB:212:GLN:CD    | 2:QB:212:GLN:C     | 2.82                     | 0.48              |
| 3:QC:14:ILE:C      | 3:QC:16:ARG:H      | 2.21                     | 0.48              |
| 4:QD:163:GLU:O     | 4:QD:165:MET:N     | 2.46                     | 0.48              |
| 5:QE:10:MET:HB2    | 5:QE:32:VAL:HG22   | 1.94                     | 0.48              |
| 11:QK:19:ALA:CA    | 11:QK:32:ILE:HG22  | 2.43                     | 0.48              |
| 11:QK:34:ASP:HB2   | 11:QK:35:PRO:HD2   | 1.95                     | 0.48              |
| 13:QM:73:GLU:O     | 13:QM:76:ALA:HB3   | 2.13                     | 0.48              |
| 19:QS:24:ALA:O     | 19:QS:25:LYS:HB2   | 2.13                     | 0.48              |
| 25:RA:34:C:H41     | 25:RA:447:A:H61    | 1.60                     | 0.48              |
| 25:RA:1839:G:C8    | 25:RA:1927:A:H1'   | 2.49                     | 0.48              |
| 28:RE:77:ILE:CD1   | 28:RE:78:LEU:N     | 2.70                     | 0.48              |
| 29:RF:107:LYS:O    | 29:RF:110:LEU:N    | 2.47                     | 0.48              |
| 29:RF:144:LYS:C    | 29:RF:146:ALA:H    | 2.21                     | 0.48              |
| 29:RF:155:LEU:HA   | 29:RF:174:VAL:HG12 | 1.95                     | 0.48              |
| 30:RG:16:ARG:HB3   | 30:RG:17:PRO:HD3   | 1.94                     | 0.48              |
| 34:RO:1:MET:HE3    | 34:RO:67:LYS:HG2   | 1.95                     | 0.48              |
| 35:RP:112:LEU:HD12 | 35:RP:127:ALA:CB   | 2.44                     | 0.48              |
| 35:RP:144:GLU:OE1  | 35:RP:144:GLU:O    | 2.31                     | 0.48              |
| 36:RQ:34:LEU:HD23  | 36:RQ:104:PHE:HD1  | 1.77                     | 0.48              |
| 37:RR:61:HIS:O     | 37:RR:65:LEU:HD13  | 2.14                     | 0.48              |
| 38:RS:46:VAL:HG12  | 38:RS:47:THR:N     | 2.28                     | 0.48              |
| 38:RS:59:LYS:HG2   | 38:RS:60:GLY:N     | 2.13                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:RX:14:SER:O    | 43:RX:15:GLU:C     | 2.57                     | 0.48              |
| 47:R1:92:LYS:O    | 47:R1:93:GLU:C     | 2.56                     | 0.48              |
| 54:R8:41:ILE:HG13 | 54:R8:42:ARG:N     | 2.28                     | 0.48              |
| 1:XA:375:U:H4'    | 16:XP:17:TYR:CE2   | 2.40                     | 0.48              |
| 1:XA:1231:G:O3'   | 9:XI:126:SER:OG    | 2.31                     | 0.48              |
| 3:XC:148:GLY:O    | 3:XC:202:ILE:HA    | 2.14                     | 0.48              |
| 3:XC:153:VAL:HA   | 3:XC:197:GLY:O     | 2.13                     | 0.48              |
| 4:XD:6:GLY:O      | 4:XD:8:VAL:HG23    | 2.14                     | 0.48              |
| 4:XD:154:ASN:O    | 4:XD:155:LEU:O     | 2.32                     | 0.48              |
| 4:XD:196:LEU:HB3  | 4:XD:197:PRO:HD2   | 1.95                     | 0.48              |
| 5:XE:11:ILE:CG1   | 5:XE:31:LEU:HD12   | 2.42                     | 0.48              |
| 5:XE:96:PRO:HA    | 5:XE:117:ASP:OD2   | 2.14                     | 0.48              |
| 7:XG:60:LYS:O     | 7:XG:61:VAL:C      | 2.57                     | 0.48              |
| 8:XH:86:ILE:HG13  | 8:XH:133:LEU:CD2   | 2.44                     | 0.48              |
| 15:XO:24:SER:OG   | 15:XO:25:THR:N     | 2.47                     | 0.48              |
| 25:YA:1899:G:H21  | 25:YA:1902:C:N4    | 2.12                     | 0.48              |
| 25:YA:2370:G:C6   | 25:YA:2371:G:C6    | 3.01                     | 0.48              |
| 28:YE:23:VAL:HG12 | 28:YE:173:VAL:HG21 | 1.94                     | 0.48              |
| 28:YE:38:THR:O    | 28:YE:42:ASP:HB2   | 2.13                     | 0.48              |
| 31:YH:7:LEU:N     | 31:YH:8:PRO:CD     | 2.77                     | 0.48              |
| 31:YH:53:GLU:CD   | 31:YH:54:ARG:H     | 2.21                     | 0.48              |
| 31:YH:119:GLU:CD  | 31:YH:120:GLY:H    | 2.22                     | 0.48              |
| 32:YI:83:ALA:O    | 32:YI:85:GLU:N     | 2.47                     | 0.48              |
| 32:YI:104:GLN:C   | 32:YI:105:HIS:HD1  | 2.21                     | 0.48              |
| 36:YQ:19:GLY:O    | 36:YQ:98:LYS:HD3   | 2.14                     | 0.48              |
| 36:YQ:31:ASP:O    | 36:YQ:32:TYR:CG    | 2.66                     | 0.48              |
| 37:YR:42:LYS:HA   | 37:YR:45:ARG:HD2   | 1.95                     | 0.48              |
| 37:YR:48:VAL:O    | 37:YR:49:ASP:C     | 2.57                     | 0.48              |
| 43:YX:35:THR:O    | 43:YX:36:LYS:C     | 2.55                     | 0.48              |
| 43:YX:44:GLU:OE1  | 43:YX:50:LYS:HD2   | 2.13                     | 0.48              |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HD23 | 1.95                     | 0.48              |
| 50:Y4:42:PHE:O    | 50:Y4:44:THR:O     | 2.31                     | 0.48              |
| 52:Y6:41:PRO:HD2  | 52:Y6:46:HIS:H     | 1.77                     | 0.48              |
| 1:QA:1305:G:O2'   | 1:QA:1306:A:H8     | 1.97                     | 0.48              |
| 1:QA:1344:C:HO2'  | 1:QA:1348:U:HO2'   | 1.57                     | 0.48              |
| 3:QC:71:ALA:HA    | 3:QC:106:VAL:HB    | 1.94                     | 0.48              |
| 8:QH:45:ILE:O     | 8:QH:45:ILE:HG13   | 2.13                     | 0.48              |
| 8:QH:109:ILE:HG12 | 8:QH:110:ALA:N     | 2.27                     | 0.48              |
| 12:QL:22:SER:C    | 12:QL:24:VAL:H     | 2.22                     | 0.48              |
| 19:QS:42:PRO:CG   | 50:R4:63:TYR:HE2   | 2.26                     | 0.48              |
| 25:RA:96:G:H4'    | 48:R2:48:HIS:NE2   | 2.29                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:847:U:H3     | 25:RA:934:G:N2    | 2.10                     | 0.48              |
| 25:RA:2335:A:O2'   | 25:RA:2336:A:O5'  | 2.31                     | 0.48              |
| 27:RD:48:ARG:HG3   | 27:RD:48:ARG:HH11 | 1.78                     | 0.48              |
| 30:RG:136:ARG:O    | 30:RG:154:GLY:CA  | 2.62                     | 0.48              |
| 31:RH:7:LEU:N      | 31:RH:8:PRO:CD    | 2.77                     | 0.48              |
| 33:RN:103:VAL:O    | 33:RN:104:LYS:C   | 2.56                     | 0.48              |
| 35:RP:71:VAL:HG13  | 35:RP:72:PRO:CD   | 2.43                     | 0.48              |
| 35:RP:138:LEU:HD11 | 35:RP:144:GLU:CG  | 2.42                     | 0.48              |
| 36:RQ:19:GLY:O     | 36:RQ:98:LYS:HD3  | 2.14                     | 0.48              |
| 39:RT:57:PHE:O     | 39:RT:59:THR:N    | 2.46                     | 0.48              |
| 44:RY:57:GLN:O     | 44:RY:58:GLY:O    | 2.32                     | 0.48              |
| 1:XA:1077:G:N2     | 1:XA:1080:A:OP2   | 2.27                     | 0.48              |
| 1:XA:1322:C:OP2    | 19:XS:78:ARG:NH2  | 2.46                     | 0.48              |
| 3:XC:195:VAL:CG1   | 3:XC:196:LEU:H    | 2.27                     | 0.48              |
| 4:XD:114:ARG:HH11  | 4:XD:114:ARG:CG   | 2.17                     | 0.48              |
| 7:XG:97:GLN:O      | 7:XG:101:LEU:HG   | 2.14                     | 0.48              |
| 11:XK:19:ALA:CB    | 11:XK:32:ILE:HG22 | 2.42                     | 0.48              |
| 13:XM:7:VAL:HG21   | 30:YG:113:ARG:O   | 2.13                     | 0.48              |
| 16:XP:25:ARG:HG3   | 16:XP:25:ARG:HH11 | 1.79                     | 0.48              |
| 20:XT:30:LYS:O     | 20:XT:33:ILE:HG12 | 2.14                     | 0.48              |
| 20:XT:44:ALA:C     | 20:XT:91:LEU:HB3  | 2.39                     | 0.48              |
| 26:YB:89:G:H8      | 26:YB:89:G:OP2    | 1.96                     | 0.48              |
| 27:YD:35:LYS:CG    | 27:YD:64:ILE:CG2  | 2.92                     | 0.48              |
| 27:YD:35:LYS:HD2   | 27:YD:104:TYR:CE1 | 2.49                     | 0.48              |
| 30:YG:125:PHE:HB3  | 30:YG:166:ASP:HB2 | 1.95                     | 0.48              |
| 31:YH:124:GLU:HB3  | 31:YH:132:ARG:CD  | 2.44                     | 0.48              |
| 38:YS:18:ILE:O     | 38:YS:19:LYS:O    | 2.31                     | 0.48              |
| 38:YS:66:ALA:HA    | 38:YS:69:VAL:HG12 | 1.96                     | 0.48              |
| 39:YT:105:LEU:C    | 39:YT:107:ASP:OD1 | 2.56                     | 0.48              |
| 48:Y2:33:MET:O     | 48:Y2:37:PHE:HD1  | 1.95                     | 0.48              |
| 48:Y2:69:ARG:HH11  | 48:Y2:69:ARG:HB3  | 1.79                     | 0.48              |
| 50:Y4:8:LYS:O      | 50:Y4:9:LEU:CB    | 2.62                     | 0.48              |
| 1:QA:15:G:H4'      | 5:QE:24:ARG:HH12  | 1.78                     | 0.48              |
| 1:QA:224:C:H2'     | 1:QA:225:C:C6     | 2.49                     | 0.48              |
| 1:QA:352:C:O2'     | 1:QA:353:A:O5'    | 2.31                     | 0.48              |
| 1:QA:1148:U:H2'    | 1:QA:1149:C:O4'   | 2.13                     | 0.48              |
| 1:QA:1226:C:O2'    | 13:QM:103:THR:O   | 2.23                     | 0.48              |
| 3:QC:153:VAL:HA    | 3:QC:197:GLY:O    | 2.13                     | 0.48              |
| 4:QD:165:MET:CE    | 4:QD:168:ARG:HD2  | 2.44                     | 0.48              |
| 5:QE:62:ALA:C      | 5:QE:64:ARG:H     | 2.21                     | 0.48              |
| 7:QG:60:LYS:O      | 7:QG:61:VAL:C     | 2.57                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:QK:20:TYR:C     | 11:QK:21:ILE:HD12  | 2.38                     | 0.48              |
| 12:QL:10:LEU:CB    | 17:QQ:32:TYR:CE2   | 2.97                     | 0.48              |
| 25:RA:51:G:H8      | 25:RA:51:G:OP2     | 1.97                     | 0.48              |
| 25:RA:270(U):C:H2' | 25:RA:270(V):G:C8  | 2.49                     | 0.48              |
| 25:RA:1637:A:H5'   | 25:RA:1760:A:O2'   | 2.14                     | 0.48              |
| 25:RA:1678:G:H22   | 25:RA:1989:G:N2    | 2.10                     | 0.48              |
| 25:RA:1930:G:O2'   | 25:RA:1931:U:O5'   | 2.32                     | 0.48              |
| 28:RE:61:ARG:CB    | 28:RE:62:PRO:CD    | 2.90                     | 0.48              |
| 28:RE:93:VAL:H     | 28:RE:95:ILE:CD1   | 2.23                     | 0.48              |
| 29:RF:34:TRP:HD1   | 35:RP:6:LEU:HB3    | 1.79                     | 0.48              |
| 29:RF:51:THR:O     | 29:RF:93:LYS:NZ    | 2.38                     | 0.48              |
| 30:RG:3:LEU:HD21   | 50:R4:25:TYR:CE1   | 2.48                     | 0.48              |
| 33:RN:34:LEU:O     | 33:RN:49:GLY:HA3   | 2.13                     | 0.48              |
| 36:RQ:21:THR:HB    | 36:RQ:22:LYS:H     | 1.42                     | 0.48              |
| 38:RS:55:ALA:O     | 38:RS:56:LEU:HB3   | 2.13                     | 0.48              |
| 44:RY:11:ASP:HB2   | 44:RY:27:VAL:HG11  | 1.94                     | 0.48              |
| 47:R1:56:GLN:NE2   | 47:R1:56:GLN:H     | 2.10                     | 0.48              |
| 50:R4:60:GLN:O     | 50:R4:63:TYR:HB3   | 2.13                     | 0.48              |
| 51:R5:49:CYS:SG    | 51:R5:58:LEU:HB2   | 2.53                     | 0.48              |
| 55:R9:1:MET:HE2    | 55:R9:10:ILE:HD13  | 1.95                     | 0.48              |
| 1:XA:595:G:H1'     | 1:XA:596:C:H5      | 1.78                     | 0.48              |
| 2:XB:193:ASP:OD2   | 2:XB:196:LEU:CG    | 2.58                     | 0.48              |
| 2:XB:212:GLN:CD    | 2:XB:212:GLN:C     | 2.82                     | 0.48              |
| 4:XD:60:GLU:O      | 4:XD:63:LYS:HB3    | 2.14                     | 0.48              |
| 5:XE:78:HIS:CE1    | 5:XE:142:LEU:HD23  | 2.48                     | 0.48              |
| 5:XE:84:PHE:HD2    | 5:XE:130:ASN:O     | 1.97                     | 0.48              |
| 5:XE:100:VAL:O     | 5:XE:107:ARG:NH2   | 2.47                     | 0.48              |
| 6:XF:79:LEU:O      | 6:XF:85:VAL:HG11   | 2.14                     | 0.48              |
| 8:XH:44:PHE:CD1    | 8:XH:80:ILE:HG12   | 2.49                     | 0.48              |
| 9:XI:59:PHE:CZ     | 9:XI:88:TYR:CE1    | 3.01                     | 0.48              |
| 10:XJ:74:ILE:HG12  | 10:XJ:74:ILE:O     | 2.14                     | 0.48              |
| 12:XL:22:SER:C     | 12:XL:24:VAL:H     | 2.22                     | 0.48              |
| 14:XN:15:LYS:HD2   | 14:XN:16:PHE:CE2   | 2.49                     | 0.48              |
| 16:XP:34:GLU:HG2   | 16:XP:35:LYS:N     | 2.29                     | 0.48              |
| 21:XU:15:ARG:HG2   | 21:XU:15:ARG:NH1   | 2.28                     | 0.48              |
| 25:YA:987:G:O2'    | 25:YA:1000:A:N3    | 2.42                     | 0.48              |
| 25:YA:1019:U:H3    | 25:YA:1142(A):A:N6 | 2.05                     | 0.48              |
| 25:YA:1543:A:HO2'  | 25:YA:1544:C:P     | 2.36                     | 0.48              |
| 25:YA:2377:A:H4'   | 38:YS:111:GLU:O    | 2.14                     | 0.48              |
| 27:YD:198:ASN:C    | 27:YD:198:ASN:ND2  | 2.69                     | 0.48              |
| 28:YE:55:ASN:O     | 28:YE:57:LYS:N     | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:HD2 | 1.78                     | 0.48              |
| 33:YN:103:VAL:O   | 33:YN:104:LYS:C   | 2.57                     | 0.48              |
| 35:YP:35:HIS:O    | 35:YP:36:LYS:O    | 2.31                     | 0.48              |
| 37:YR:44:LEU:HD22 | 37:YR:48:VAL:CG2  | 2.43                     | 0.48              |
| 39:YT:96:ARG:NH1  | 39:YT:96:ARG:CB   | 2.77                     | 0.48              |
| 42:YW:34:ASN:O    | 42:YW:35:ILE:C    | 2.55                     | 0.48              |
| 43:YX:6:ASP:OD1   | 48:Y2:29:LYS:NZ   | 2.46                     | 0.48              |
| 45:YZ:166:SER:HB2 | 45:YZ:167:PRO:C   | 2.39                     | 0.48              |
| 46:Y0:11:ARG:CZ   | 46:Y0:11:ARG:HB3  | 2.42                     | 0.48              |
| 52:Y6:8:LYS:O     | 52:Y6:27:LYS:HA   | 2.13                     | 0.48              |
| 1:QA:1081:G:OP1   | 5:QE:16:THR:OG1   | 2.32                     | 0.48              |
| 1:QA:1322:C:O2'   | 1:QA:1323:G:H5'   | 2.13                     | 0.48              |
| 1:QA:1388:C:H2'   | 1:QA:1389:C:H6    | 1.78                     | 0.48              |
| 4:QD:153:ARG:CZ   | 4:QD:181:MET:HG3  | 2.44                     | 0.48              |
| 5:QE:84:PHE:HD2   | 5:QE:130:ASN:O    | 1.97                     | 0.48              |
| 8:QH:86:ILE:HG12  | 8:QH:135:CYS:HA   | 1.96                     | 0.48              |
| 9:QI:17:VAL:HG11  | 9:QI:81:ILE:HA    | 1.96                     | 0.48              |
| 11:QK:41:THR:HG22 | 11:QK:42:TRP:N    | 2.28                     | 0.48              |
| 11:QK:48:ILE:HG21 | 11:QK:63:LEU:HD13 | 1.96                     | 0.48              |
| 12:QL:127:GLU:O   | 12:QL:128:ALA:CB  | 2.62                     | 0.48              |
| 16:QP:21:VAL:HG23 | 16:QP:34:GLU:H    | 1.79                     | 0.48              |
| 16:QP:57:ARG:HG3  | 16:QP:57:ARG:HH11 | 1.79                     | 0.48              |
| 16:QP:60:LEU:CA   | 16:QP:64:ALA:HB3  | 2.43                     | 0.48              |
| 16:QP:71:ARG:HH11 | 16:QP:71:ARG:HB2  | 1.79                     | 0.48              |
| 17:QQ:3:LYS:HD2   | 17:QQ:60:ILE:HD11 | 1.95                     | 0.48              |
| 21:QU:9:ARG:HH11  | 21:QU:9:ARG:HG2   | 1.78                     | 0.48              |
| 25:RA:1359:A:OP2  | 25:RA:1371:G:N2   | 2.36                     | 0.48              |
| 25:RA:1384:A:H1'  | 25:RA:1405:U:O4'  | 2.14                     | 0.48              |
| 25:RA:2405:G:H1'  | 25:RA:2412:A:N6   | 2.29                     | 0.48              |
| 25:RA:2467:C:H4'  | 36:RQ:123:HIS:CD2 | 2.49                     | 0.48              |
| 27:RD:130:ALA:HA  | 27:RD:192:THR:HA  | 1.96                     | 0.48              |
| 33:RN:82:LEU:HD12 | 33:RN:83:LYS:N    | 2.27                     | 0.48              |
| 37:RR:63:ARG:NH1  | 37:RR:63:ARG:HG3  | 2.29                     | 0.48              |
| 40:RU:79:PHE:HE2  | 40:RU:83:LEU:CD2  | 2.26                     | 0.48              |
| 54:R8:40:GLU:O    | 54:R8:41:ILE:C    | 2.56                     | 0.48              |
| 1:XA:192:U:H2'    | 1:XA:193:C:C6     | 2.49                     | 0.48              |
| 2:XB:214:ILE:O    | 2:XB:218:ALA:HB2  | 2.13                     | 0.48              |
| 5:XE:87:SER:HB3   | 5:XE:131:ILE:HD13 | 1.95                     | 0.48              |
| 9:XI:7:THR:O      | 9:XI:83:ARG:HD2   | 2.14                     | 0.48              |
| 11:XK:82:VAL:O    | 11:XK:108:ILE:HA  | 2.13                     | 0.48              |
| 13:XM:69:GLU:O    | 13:XM:70:LEU:C    | 2.56                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:XQ:74:LEU:HD12  | 17:XQ:75:ARG:NE    | 2.28                     | 0.48              |
| 25:YA:270(G):C:H2' | 25:YA:270(H):C:H6  | 1.78                     | 0.48              |
| 25:YA:442:G:O4'    | 29:YF:46:ARG:HD3   | 2.13                     | 0.48              |
| 27:YD:130:ALA:HA   | 27:YD:192:THR:HA   | 1.95                     | 0.48              |
| 29:YF:34:TRP:HD1   | 35:YP:6:LEU:HB3    | 1.79                     | 0.48              |
| 29:YF:45:ARG:HG2   | 29:YF:45:ARG:NH1   | 2.28                     | 0.48              |
| 29:YF:129:PHE:CD2  | 29:YF:163:VAL:HG21 | 2.48                     | 0.48              |
| 30:YG:111:LEU:HD22 | 30:YG:120:LEU:HD21 | 1.96                     | 0.48              |
| 31:YH:120:GLY:HA3  | 31:YH:140:LYS:NZ   | 2.27                     | 0.48              |
| 33:YN:34:LEU:O     | 33:YN:49:GLY:HA3   | 2.13                     | 0.48              |
| 33:YN:63:THR:HG22  | 33:YN:66:LYS:HZ1   | 1.78                     | 0.48              |
| 33:YN:118:LYS:C    | 33:YN:120:LEU:H    | 2.20                     | 0.48              |
| 36:YQ:42:ILE:HD12  | 36:YQ:42:ILE:N     | 2.29                     | 0.48              |
| 39:YT:16:ARG:NE    | 39:YT:19:LEU:HD21  | 2.27                     | 0.48              |
| 40:YU:79:PHE:HE2   | 40:YU:83:LEU:CD2   | 2.27                     | 0.48              |
| 47:Y1:76:ARG:HD2   | 47:Y1:76:ARG:N     | 2.29                     | 0.48              |
| 47:Y1:92:LYS:O     | 47:Y1:93:GLU:C     | 2.56                     | 0.48              |
| 48:Y2:27:GLU:H     | 48:Y2:27:GLU:CD    | 2.17                     | 0.48              |
| 53:Y7:32:LYS:O     | 53:Y7:33:ARG:C     | 2.55                     | 0.48              |
| 1:QA:1129:C:H4'    | 1:QA:1130:A:H8     | 1.79                     | 0.48              |
| 1:QA:1301:U:O2     | 1:QA:1301:U:H2'    | 2.14                     | 0.48              |
| 2:QB:24:TRP:CD1    | 2:QB:26:PRO:HD3    | 2.49                     | 0.48              |
| 2:QB:24:TRP:CZ3    | 2:QB:26:PRO:HA     | 2.49                     | 0.48              |
| 2:QB:33:TYR:C      | 2:QB:33:TYR:CD1    | 2.92                     | 0.48              |
| 4:QD:3:ARG:O       | 4:QD:5:ILE:HG13    | 2.14                     | 0.48              |
| 7:QG:51:GLN:HA     | 7:QG:51:GLN:OE1    | 2.14                     | 0.48              |
| 7:QG:79:ARG:O      | 7:QG:80:VAL:HG23   | 2.14                     | 0.48              |
| 7:QG:97:GLN:O      | 7:QG:101:LEU:HG    | 2.14                     | 0.48              |
| 8:QH:6:ILE:O       | 8:QH:10:LEU:HG     | 2.14                     | 0.48              |
| 10:QJ:4:ILE:CB     | 10:QJ:74:ILE:HD11  | 2.36                     | 0.48              |
| 11:QK:13:GLN:HG3   | 11:QK:75:TYR:O     | 2.14                     | 0.48              |
| 12:QL:120:TYR:O    | 12:QL:121:GLY:C    | 2.57                     | 0.48              |
| 13:QM:12:ASN:O     | 13:QM:13:LYS:HB2   | 2.13                     | 0.48              |
| 15:QO:83:GLU:C     | 15:QO:85:LEU:N     | 2.71                     | 0.48              |
| 18:QR:31:LEU:HD23  | 18:QR:31:LEU:N     | 2.29                     | 0.48              |
| 19:QS:9:VAL:O      | 19:QS:10:PHE:HB3   | 2.13                     | 0.48              |
| 25:RA:128:C:H2'    | 25:RA:129:C:C6     | 2.49                     | 0.48              |
| 25:RA:335:C:H4'    | 44:RY:73:ARG:CZ    | 2.44                     | 0.48              |
| 25:RA:345:A:H1'    | 25:RA:346:A:N7     | 2.29                     | 0.48              |
| 25:RA:965:C:H4'    | 25:RA:2273:A:H1'   | 1.95                     | 0.48              |
| 25:RA:1138:G:O3'   | 33:RN:101:HIS:HE1  | 1.97                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2327:A:H2'   | 25:RA:2328:A:C8    | 2.48                     | 0.48              |
| 25:RA:2853:C:H2'   | 25:RA:2854:G:C8    | 2.49                     | 0.48              |
| 26:RB:16:G:H2'     | 26:RB:17:C:C6      | 2.49                     | 0.48              |
| 26:RB:42:C:O2      | 30:RG:92:VAL:HA    | 2.14                     | 0.48              |
| 30:RG:12:TYR:O     | 30:RG:16:ARG:HB3   | 2.14                     | 0.48              |
| 30:RG:106:LEU:HA   | 30:RG:110:ALA:HB3  | 1.95                     | 0.48              |
| 31:RH:131:VAL:HG12 | 31:RH:132:ARG:N    | 2.29                     | 0.48              |
| 33:RN:96:GLU:O     | 33:RN:97:ARG:C     | 2.57                     | 0.48              |
| 34:RO:8:LEU:HB2    | 34:RO:19:ILE:CD1   | 2.43                     | 0.48              |
| 36:RQ:42:ILE:HD12  | 36:RQ:42:ILE:N     | 2.29                     | 0.48              |
| 41:RV:35:LEU:O     | 41:RV:37:VAL:N     | 2.47                     | 0.48              |
| 1:XA:1313:U:OP2    | 50:Y4:67:TYR:OH    | 2.15                     | 0.48              |
| 1:XA:1513:A:H2'    | 1:XA:1514:C:C6     | 2.49                     | 0.48              |
| 2:XB:5:ILE:O       | 2:XB:6:THR:O       | 2.32                     | 0.48              |
| 2:XB:24:TRP:CD1    | 2:XB:26:PRO:HD3    | 2.49                     | 0.48              |
| 2:XB:33:TYR:C      | 2:XB:33:TYR:CD1    | 2.92                     | 0.48              |
| 3:XC:101:LEU:HD23  | 3:XC:101:LEU:C     | 2.38                     | 0.48              |
| 4:XD:100:ARG:CZ    | 4:XD:137:SER:HA    | 2.44                     | 0.48              |
| 5:XE:72:GLN:C      | 5:XE:74:GLY:H      | 2.22                     | 0.48              |
| 5:XE:75:THR:HG23   | 5:XE:76:ILE:O      | 2.14                     | 0.48              |
| 7:XG:79:ARG:O      | 7:XG:80:VAL:HG23   | 2.14                     | 0.48              |
| 9:XI:22:GLY:O      | 9:XI:23:ASN:C      | 2.57                     | 0.48              |
| 10:XJ:47:PHE:CE1   | 10:XJ:63:PHE:HB2   | 2.32                     | 0.48              |
| 13:XM:72:ALA:O     | 13:XM:76:ALA:HB2   | 2.14                     | 0.48              |
| 17:XQ:63:ARG:HG2   | 17:XQ:64:PRO:N     | 2.28                     | 0.48              |
| 19:XS:36:ARG:HB3   | 19:XS:36:ARG:NH1   | 2.29                     | 0.48              |
| 25:YA:747:U:N1     | 51:Y5:2:ALA:HB3    | 2.29                     | 0.48              |
| 25:YA:1790:C:H5''  | 25:YA:1791:A:OP1   | 2.13                     | 0.48              |
| 25:YA:1815:A:OP2   | 27:YD:54:ARG:NH2   | 2.47                     | 0.48              |
| 27:YD:12:SER:C     | 27:YD:14:ARG:N     | 2.70                     | 0.48              |
| 27:YD:27:THR:O     | 27:YD:29:PRO:CD    | 2.62                     | 0.48              |
| 27:YD:33:LEU:HB3   | 27:YD:34:VAL:H     | 1.49                     | 0.48              |
| 28:YE:77:ILE:CD1   | 28:YE:78:LEU:N     | 2.70                     | 0.48              |
| 29:YF:155:LEU:HA   | 29:YF:174:VAL:HG12 | 1.95                     | 0.48              |
| 30:YG:97:ASP:N     | 30:YG:100:TRP:HD1  | 2.05                     | 0.48              |
| 31:YH:41:MET:HG3   | 31:YH:54:ARG:HA    | 1.96                     | 0.48              |
| 33:YN:90:MET:O     | 33:YN:91:LEU:C     | 2.57                     | 0.48              |
| 33:YN:137:LYS:CG   | 33:YN:138:LEU:H    | 2.27                     | 0.48              |
| 36:YQ:83:MET:HB2   | 46:Y0:7:LEU:HD22   | 1.95                     | 0.48              |
| 39:YT:94:ALA:O     | 39:YT:95:ARG:CB    | 2.61                     | 0.48              |
| 40:YU:79:PHE:HE2   | 40:YU:83:LEU:HD22  | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:YV:21:ARG:HD2   | 41:YV:91:TYR:CZ    | 2.49                     | 0.48              |
| 41:YV:38:LEU:HD23  | 41:YV:39:LEU:H     | 1.79                     | 0.48              |
| 43:YX:11:PRO:HB3   | 43:YX:92:LEU:CD2   | 2.43                     | 0.48              |
| 44:YY:57:GLN:O     | 44:YY:58:GLY:O     | 2.32                     | 0.48              |
| 47:Y1:94:LEU:O     | 47:Y1:95:LEU:CB    | 2.62                     | 0.48              |
| 51:Y5:3:LYS:O      | 51:Y5:4:HIS:C      | 2.56                     | 0.48              |
| 52:Y6:20:ASN:ND2   | 52:Y6:42:TRP:CZ2   | 2.82                     | 0.48              |
| 1:QA:184:G:H2'     | 1:QA:185:A:C8      | 2.45                     | 0.47              |
| 1:QA:986:A:N3      | 19:QS:52:TYR:OH    | 2.46                     | 0.47              |
| 1:QA:1064:G:HO2'   | 1:QA:1065:U:P      | 2.36                     | 0.47              |
| 2:QB:87:ARG:NH1    | 2:QB:220:ASP:OD1   | 2.46                     | 0.47              |
| 2:QB:97:TRP:HZ2    | 2:QB:102:LEU:HD13  | 1.78                     | 0.47              |
| 2:QB:109:SER:C     | 2:QB:111:ARG:H     | 2.21                     | 0.47              |
| 5:QE:75:THR:HG23   | 5:QE:76:ILE:O      | 2.14                     | 0.47              |
| 7:QG:63:LYS:O      | 7:QG:63:LYS:HD2    | 2.13                     | 0.47              |
| 8:QH:44:PHE:CD1    | 8:QH:80:ILE:HG12   | 2.49                     | 0.47              |
| 9:QI:7:THR:O       | 9:QI:83:ARG:HD2    | 2.14                     | 0.47              |
| 9:QI:22:GLY:HA3    | 9:QI:60:ASP:OD2    | 2.13                     | 0.47              |
| 9:QI:33:PHE:HZ     | 9:QI:47:LEU:HD21   | 1.76                     | 0.47              |
| 10:QJ:39:PRO:CB    | 10:QJ:70:ARG:HH12  | 2.27                     | 0.47              |
| 13:QM:50:GLU:O     | 13:QM:54:VAL:HG23  | 2.13                     | 0.47              |
| 17:QQ:33:GLY:O     | 17:QQ:34:LYS:C     | 2.55                     | 0.47              |
| 20:QT:37:SER:HB3   | 20:QT:84:LEU:CD2   | 2.44                     | 0.47              |
| 20:QT:44:ALA:C     | 20:QT:91:LEU:HB3   | 2.39                     | 0.47              |
| 20:QT:50:GLU:HA    | 20:QT:100:ILE:CG2  | 2.44                     | 0.47              |
| 25:RA:270(S):G:C1' | 47:R1:78:LYS:HD2   | 2.43                     | 0.47              |
| 25:RA:824:A:H1'    | 25:RA:2358:G:N7    | 2.29                     | 0.47              |
| 25:RA:1043:C:H42   | 25:RA:1112:G:H1    | 1.62                     | 0.47              |
| 25:RA:2688:U:H5    | 25:RA:2720:U:OP2   | 1.95                     | 0.47              |
| 27:RD:35:LYS:CG    | 27:RD:64:ILE:CG2   | 2.92                     | 0.47              |
| 28:RE:69:LYS:C     | 28:RE:71:GLY:N     | 2.71                     | 0.47              |
| 28:RE:120:TRP:O    | 28:RE:121:ASN:HB2  | 2.14                     | 0.47              |
| 28:RE:203:LYS:HD2  | 28:RE:203:LYS:C    | 2.39                     | 0.47              |
| 33:RN:57:ALA:O     | 33:RN:58:ASP:CB    | 2.61                     | 0.47              |
| 33:RN:90:MET:O     | 33:RN:91:LEU:C     | 2.57                     | 0.47              |
| 33:RN:113:GLY:O    | 33:RN:116:LEU:HB2  | 2.14                     | 0.47              |
| 38:RS:105:ALA:C    | 38:RS:110:LEU:HD21 | 2.38                     | 0.47              |
| 42:RW:66:GLU:O     | 42:RW:69:LEU:HG    | 2.14                     | 0.47              |
| 44:RY:56:PRO:O     | 44:RY:58:GLY:N     | 2.47                     | 0.47              |
| 47:R1:8:SER:OG     | 47:R1:10:LYS:HG3   | 2.13                     | 0.47              |
| 53:R7:32:LYS:O     | 53:R7:33:ARG:C     | 2.56                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1190:G:OP1    | 3:XC:5:ILE:HD12    | 2.14                     | 0.47              |
| 4:XD:198:VAL:CG1   | 4:XD:199:ASN:N     | 2.75                     | 0.47              |
| 8:XH:86:ILE:HG22   | 8:XH:87:SER:N      | 2.29                     | 0.47              |
| 11:XK:20:TYR:C     | 11:XK:21:ILE:HD12  | 2.38                     | 0.47              |
| 11:XK:110:ASP:HB2  | 18:XR:88:LYS:HD3   | 1.95                     | 0.47              |
| 12:XL:61:THR:O     | 12:XL:63:GLY:N     | 2.45                     | 0.47              |
| 14:XN:6:LEU:HD22   | 14:XN:23:ARG:NH2   | 2.29                     | 0.47              |
| 20:XT:101:GLY:C    | 20:XT:103:GLY:H    | 2.22                     | 0.47              |
| 25:YA:264:C:C2'    | 25:YA:265:A:H5''   | 2.44                     | 0.47              |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:C8  | 2.49                     | 0.47              |
| 25:YA:628:G:H2'    | 25:YA:629:G:C8     | 2.48                     | 0.47              |
| 25:YA:1162:G:H1'   | 41:YV:23:GLU:OE2   | 2.14                     | 0.47              |
| 25:YA:1416:G:H2'   | 25:YA:1417:C:H6    | 1.78                     | 0.47              |
| 25:YA:1695:G:H1'   | 27:YD:8:PRO:O      | 2.14                     | 0.47              |
| 25:YA:2415:G:H4'   | 35:YP:66:GLY:C     | 2.39                     | 0.47              |
| 25:YA:2790:A:H2'   | 25:YA:2791:C:H5''  | 1.96                     | 0.47              |
| 28:YE:15:PHE:CD1   | 28:YE:20:ALA:HB2   | 2.49                     | 0.47              |
| 31:YH:45:VAL:O     | 31:YH:45:VAL:HG13  | 2.14                     | 0.47              |
| 31:YH:127:GLU:HB3  | 31:YH:128:PRO:HD2  | 1.93                     | 0.47              |
| 32:YI:13:GLY:HA3   | 32:YI:17:GLN:CD    | 2.39                     | 0.47              |
| 34:YO:107:ARG:NH1  | 39:YT:36:GLU:OE1   | 2.46                     | 0.47              |
| 36:YQ:60:ARG:NH2   | 36:YQ:60:ARG:HB2   | 2.28                     | 0.47              |
| 36:YQ:83:MET:H     | 46:Y0:7:LEU:HD22   | 1.80                     | 0.47              |
| 38:YS:105:ALA:C    | 38:YS:110:LEU:HD21 | 2.38                     | 0.47              |
| 40:YU:53:ARG:C     | 40:YU:55:ARG:H     | 2.20                     | 0.47              |
| 42:YW:30:GLU:O     | 42:YW:34:ASN:ND2   | 2.46                     | 0.47              |
| 50:Y4:48:ARG:C     | 50:Y4:49:PHE:HD1   | 2.22                     | 0.47              |
| 50:Y4:60:GLN:O     | 50:Y4:63:TYR:HB3   | 2.14                     | 0.47              |
| 54:Y8:53:PRO:CD    | 54:Y8:54:GLU:N     | 2.77                     | 0.47              |
| 1:QA:452:A:H62     | 1:QA:480:U:H3      | 1.61                     | 0.47              |
| 1:QA:521:G:H4'     | 12:QL:73:GLU:HG3   | 1.95                     | 0.47              |
| 1:QA:973:G:O4'     | 10:QJ:55:LYS:HG2   | 2.13                     | 0.47              |
| 1:QA:1329:A:P      | 13:QM:28:ALA:HB3   | 2.54                     | 0.47              |
| 2:QB:206:ASP:HA    | 2:QB:211:ILE:HD11  | 1.94                     | 0.47              |
| 3:QC:12:LEU:C      | 3:QC:14:ILE:H      | 2.22                     | 0.47              |
| 3:QC:16:ARG:NH2    | 3:QC:183:ASP:OD2   | 2.47                     | 0.47              |
| 4:QD:6:GLY:O       | 4:QD:8:VAL:HG23    | 2.14                     | 0.47              |
| 5:QE:87:SER:HB3    | 5:QE:131:ILE:HD13  | 1.95                     | 0.47              |
| 5:QE:141:GLN:HA    | 5:QE:143:ARG:HH12  | 1.79                     | 0.47              |
| 9:QI:95:LYS:HD3    | 9:QI:95:LYS:C      | 2.39                     | 0.47              |
| 10:QJ:24:VAL:HG21  | 10:QJ:37:PRO:CG    | 2.43                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:QL:85:ILE:HD11  | 12:QL:98:TYR:CB   | 2.43                     | 0.47              |
| 13:QM:30:ALA:O     | 13:QM:33:ALA:N    | 2.47                     | 0.47              |
| 15:QO:24:SER:OG    | 15:QO:25:THR:N    | 2.47                     | 0.47              |
| 20:QT:30:LYS:O     | 20:QT:33:ILE:HG12 | 2.14                     | 0.47              |
| 20:QT:64:ASP:O     | 20:QT:67:ALA:N    | 2.47                     | 0.47              |
| 20:QT:101:GLY:C    | 20:QT:103:GLY:H   | 2.21                     | 0.47              |
| 22:QV:19:G:H4'     | 22:QV:20:U:OP2    | 2.14                     | 0.47              |
| 25:RA:2134:A:H62   | 25:RA:2157:G:H1'  | 1.80                     | 0.47              |
| 28:RE:18:ASP:O     | 28:RE:19:ARG:C    | 2.56                     | 0.47              |
| 28:RE:55:ASN:C     | 28:RE:57:LYS:N    | 2.62                     | 0.47              |
| 29:RF:183:VAL:O    | 29:RF:184:TYR:C   | 2.57                     | 0.47              |
| 31:RH:45:VAL:O     | 31:RH:45:VAL:HG13 | 2.14                     | 0.47              |
| 31:RH:124:GLU:HB3  | 31:RH:132:ARG:CD  | 2.44                     | 0.47              |
| 31:RH:154:PRO:CG   | 31:RH:162:ILE:O   | 2.61                     | 0.47              |
| 33:RN:67:LEU:O     | 33:RN:88:GLU:HG3  | 2.14                     | 0.47              |
| 33:RN:87:LEU:C     | 33:RN:87:LEU:CD2  | 2.86                     | 0.47              |
| 33:RN:131:GLN:HE21 | 33:RN:132:ALA:H   | 1.58                     | 0.47              |
| 33:RN:137:LYS:CG   | 33:RN:138:LEU:N   | 2.78                     | 0.47              |
| 35:RP:47:ASP:OD1   | 35:RP:50:ARG:NH2  | 2.47                     | 0.47              |
| 35:RP:75:ILE:H     | 35:RP:75:ILE:CD1  | 2.14                     | 0.47              |
| 36:RQ:57:HIS:ND1   | 36:RQ:58:PHE:N    | 2.62                     | 0.47              |
| 37:RR:10:LEU:O     | 37:RR:12:ARG:HG3  | 2.14                     | 0.47              |
| 37:RR:48:VAL:O     | 37:RR:49:ASP:C    | 2.57                     | 0.47              |
| 41:RV:66:ARG:NH1   | 41:RV:88:ARG:NH1  | 2.61                     | 0.47              |
| 44:RY:81:LYS:NZ    | 44:RY:98:VAL:HB   | 2.29                     | 0.47              |
| 51:R5:57:VAL:O     | 51:R5:57:VAL:HG13 | 2.14                     | 0.47              |
| 1:XA:1298:C:H4'    | 1:XA:1299:A:N9    | 2.29                     | 0.47              |
| 2:XB:96:ARG:HD2    | 2:XB:96:ARG:N     | 2.20                     | 0.47              |
| 3:XC:71:ALA:HA     | 3:XC:106:VAL:HB   | 1.95                     | 0.47              |
| 4:XD:79:PHE:HE2    | 4:XD:83:SER:HB2   | 1.79                     | 0.47              |
| 4:XD:165:MET:CE    | 4:XD:168:ARG:HD2  | 2.44                     | 0.47              |
| 5:XE:36:ASP:C      | 5:XE:37:ARG:HG2   | 2.38                     | 0.47              |
| 5:XE:153:LYS:HB2   | 5:XE:153:LYS:HZ3  | 1.79                     | 0.47              |
| 8:XH:16:ALA:HB2    | 8:XH:24:THR:CG2   | 2.44                     | 0.47              |
| 9:XI:95:LYS:HD3    | 9:XI:95:LYS:C     | 2.39                     | 0.47              |
| 11:XK:48:ILE:HG21  | 11:XK:63:LEU:HD13 | 1.96                     | 0.47              |
| 14:YN:26:ARG:NH1   | 14:YN:43:CYS:SG   | 2.86                     | 0.47              |
| 19:XS:24:ALA:O     | 19:XS:25:LYS:HB2  | 2.13                     | 0.47              |
| 20:XT:64:ASP:O     | 20:XT:67:ALA:N    | 2.47                     | 0.47              |
| 22:XV:19:G:H4'     | 22:XV:20:U:OP2    | 2.14                     | 0.47              |
| 25:YA:1682:G:H2'   | 25:YA:1683:C:C6   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2311:A:N9   | 30:YG:82:LEU:HD11  | 2.29                     | 0.47              |
| 34:YO:8:LEU:HB2   | 34:YO:19:ILE:CD1   | 2.43                     | 0.47              |
| 35:YP:47:ASP:OD1  | 35:YP:50:ARG:NH2   | 2.47                     | 0.47              |
| 35:YP:61:ARG:HH21 | 54:Y8:13:ARG:HD2   | 1.77                     | 0.47              |
| 37:YR:10:LEU:O    | 37:YR:12:ARG:HG3   | 2.14                     | 0.47              |
| 37:YR:117:VAL:O   | 37:YR:118:GLU:CB   | 2.62                     | 0.47              |
| 41:YV:2:PHE:CD2   | 41:YV:13:ARG:NH2   | 2.82                     | 0.47              |
| 41:YV:35:LEU:O    | 41:YV:37:VAL:N     | 2.47                     | 0.47              |
| 51:Y5:56:LYS:O    | 51:Y5:57:VAL:C     | 2.57                     | 0.47              |
| 53:Y7:25:PRO:HA   | 53:Y7:28:ARG:CZ    | 2.45                     | 0.47              |
| 54:Y8:41:ILE:HG13 | 54:Y8:42:ARG:N     | 2.28                     | 0.47              |
| 55:Y9:27:CYS:SG   | 55:Y9:28:GLU:N     | 2.87                     | 0.47              |
| 1:QA:244:U:H4'    | 1:QA:245:C:O5'     | 2.14                     | 0.47              |
| 1:QA:1053:G:N7    | 1:QA:1200:C:H5''   | 2.28                     | 0.47              |
| 1:QA:1399:C:C2    | 1:QA:1502:A:N6     | 2.83                     | 0.47              |
| 2:QB:33:TYR:C     | 2:QB:33:TYR:HD1    | 2.23                     | 0.47              |
| 3:QC:101:LEU:HD23 | 3:QC:101:LEU:C     | 2.38                     | 0.47              |
| 4:QD:60:GLU:O     | 4:QD:63:LYS:HB3    | 2.14                     | 0.47              |
| 4:QD:135:LEU:O    | 4:QD:137:SER:N     | 2.48                     | 0.47              |
| 5:QE:82:VAL:CG1   | 5:QE:83:GLU:H      | 2.27                     | 0.47              |
| 7:QG:69:VAL:O     | 7:QG:69:VAL:CG1    | 2.62                     | 0.47              |
| 9:QI:42:ARG:NH2   | 9:QI:75:ASP:OD2    | 2.47                     | 0.47              |
| 12:QL:27:LEU:C    | 12:QL:29:GLY:H     | 2.20                     | 0.47              |
| 14:QN:15:LYS:HD2  | 14:QN:16:PHE:CE2   | 2.49                     | 0.47              |
| 16:QP:55:ARG:O    | 16:QP:56:ALA:C     | 2.57                     | 0.47              |
| 25:RA:242:G:C5'   | 54:R8:3:LYS:HE3    | 2.44                     | 0.47              |
| 25:RA:2029:G:H2'  | 25:RA:2031:A:OP2   | 2.13                     | 0.47              |
| 25:RA:2343:C:H2'  | 25:RA:2344:U:C6    | 2.49                     | 0.47              |
| 27:RD:134:ARG:HB2 | 27:RD:135:PHE:CD2  | 2.49                     | 0.47              |
| 27:RD:145:VAL:O   | 27:RD:153:ALA:HA   | 2.15                     | 0.47              |
| 28:RE:174:ASP:O   | 28:RE:182:LEU:HD12 | 2.14                     | 0.47              |
| 31:RH:67:LEU:O    | 31:RH:71:LEU:HB2   | 2.14                     | 0.47              |
| 31:RH:82:GLY:O    | 31:RH:83:TYR:O     | 2.32                     | 0.47              |
| 33:RN:97:ARG:HA   | 33:RN:100:GLU:HB3  | 1.97                     | 0.47              |
| 35:RP:6:LEU:O     | 35:RP:7:ARG:O      | 2.31                     | 0.47              |
| 35:RP:126:VAL:HA  | 35:RP:145:PRO:HD2  | 1.95                     | 0.47              |
| 40:RU:92:ARG:CZ   | 40:RU:94:ASN:HD22  | 2.28                     | 0.47              |
| 40:RU:107:ALA:O   | 40:RU:110:VAL:HB   | 2.14                     | 0.47              |
| 41:RV:2:PHE:CD2   | 41:RV:13:ARG:NH2   | 2.83                     | 0.47              |
| 41:RV:4:ILE:HA    | 41:RV:12:TYR:O     | 2.14                     | 0.47              |
| 41:RV:16:PRO:HA   | 41:RV:96:ILE:O     | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:RY:75:ILE:HG12  | 44:RY:76:CYS:H     | 1.79                     | 0.47              |
| 44:RY:97:ARG:HG2   | 44:RY:97:ARG:NH1   | 2.28                     | 0.47              |
| 47:R1:7:ILE:HD12   | 47:R1:62:VAL:HG11  | 1.96                     | 0.47              |
| 1:XA:355:C:H1'     | 1:XA:388:G:H2'     | 1.95                     | 0.47              |
| 1:XA:1221:G:P      | 19:XS:36:ARG:HD3   | 2.54                     | 0.47              |
| 1:XA:1298:C:H4'    | 1:XA:1299:A:C4     | 2.49                     | 0.47              |
| 2:XB:4:GLU:CG      | 2:XB:5:ILE:H       | 2.00                     | 0.47              |
| 2:XB:24:TRP:CZ3    | 2:XB:26:PRO:HA     | 2.49                     | 0.47              |
| 3:XC:36:ASP:HA     | 3:XC:39:ILE:HD12   | 1.95                     | 0.47              |
| 4:XD:9:CYS:SG      | 4:XD:22:LYS:HE3    | 2.55                     | 0.47              |
| 9:XI:5:TYR:OH      | 9:XI:7:THR:HG23    | 2.15                     | 0.47              |
| 9:XI:42:ARG:NH2    | 9:XI:75:ASP:OD2    | 2.47                     | 0.47              |
| 10:XJ:24:VAL:HG21  | 10:XJ:37:PRO:CG    | 2.43                     | 0.47              |
| 11:XK:19:ALA:CA    | 11:XK:32:ILE:HG22  | 2.43                     | 0.47              |
| 12:XL:50:SER:O     | 12:XL:51:ALA:HB2   | 2.14                     | 0.47              |
| 13:XM:30:ALA:O     | 13:XM:33:ALA:N     | 2.46                     | 0.47              |
| 20:XT:50:GLU:HA    | 20:XT:100:ILE:CG2  | 2.43                     | 0.47              |
| 25:YA:219:G:H2'    | 25:YA:220:G:O4'    | 2.13                     | 0.47              |
| 25:YA:582:G:OP1    | 40:YU:14:HIS:ND1   | 2.39                     | 0.47              |
| 25:YA:1694:C:H4'   | 25:YA:1695:G:O5'   | 2.14                     | 0.47              |
| 25:YA:2389:G:H5''  | 25:YA:2390:U:O4'   | 2.14                     | 0.47              |
| 25:YA:2600:A:N7    | 27:YD:237:GLU:OE2  | 2.47                     | 0.47              |
| 25:YA:2875:C:H4'   | 39:YT:5:ALA:HB2    | 1.96                     | 0.47              |
| 28:YE:61:ARG:CB    | 28:YE:62:PRO:HD3   | 2.41                     | 0.47              |
| 31:YH:123:PHE:O    | 31:YH:125:VAL:HG23 | 2.13                     | 0.47              |
| 33:YN:57:ALA:HA    | 33:YN:60:ILE:CD1   | 2.43                     | 0.47              |
| 33:YN:57:ALA:O     | 33:YN:58:ASP:CB    | 2.62                     | 0.47              |
| 33:YN:120:LEU:HD11 | 33:YN:122:VAL:CG2  | 2.42                     | 0.47              |
| 35:YP:13:ASN:C     | 35:YP:15:ARG:H     | 2.21                     | 0.47              |
| 35:YP:107:LYS:O    | 35:YP:108:LYS:C    | 2.57                     | 0.47              |
| 37:YR:63:ARG:NH1   | 37:YR:63:ARG:HG3   | 2.29                     | 0.47              |
| 38:YS:40:ILE:HG22  | 38:YS:41:ASP:N     | 2.28                     | 0.47              |
| 41:YV:36:PRO:HA    | 41:YV:56:SER:CB    | 2.44                     | 0.47              |
| 44:YY:44:ILE:CG1   | 44:YY:45:VAL:N     | 2.70                     | 0.47              |
| 47:Y1:7:ILE:HD12   | 47:Y1:62:VAL:HG11  | 1.96                     | 0.47              |
| 54:Y8:56:GLU:O     | 54:Y8:58:ILE:N     | 2.47                     | 0.47              |
| 1:QA:368:U:OP1     | 32:YI:91:SER:OG    | 2.31                     | 0.47              |
| 1:QA:730:G:C5      | 1:QA:731:G:H1'     | 2.49                     | 0.47              |
| 1:QA:1388:C:H2'    | 1:QA:1389:C:C6     | 2.49                     | 0.47              |
| 1:QA:1435:G:H2'    | 1:QA:1436:U:C6     | 2.49                     | 0.47              |
| 2:QB:116:GLU:HA    | 2:QB:119:GLU:HB3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:QC:76:VAL:HG21  | 3:QC:103:VAL:HG11 | 1.95                     | 0.47              |
| 5:QE:96:PRO:HA    | 5:QE:117:ASP:OD2  | 2.14                     | 0.47              |
| 7:QG:107:ALA:CB   | 7:QG:134:ALA:HB2  | 2.44                     | 0.47              |
| 9:QI:9:ARG:HA     | 9:QI:76:ALA:HB1   | 1.97                     | 0.47              |
| 11:QK:124:LYS:O   | 11:QK:126:ARG:N   | 2.40                     | 0.47              |
| 13:QM:90:LEU:HA   | 13:QM:93:ARG:CD   | 2.33                     | 0.47              |
| 14:QN:6:LEU:CD2   | 14:QN:23:ARG:NH2  | 2.77                     | 0.47              |
| 18:QR:31:LEU:H    | 18:QR:31:LEU:CD2  | 2.27                     | 0.47              |
| 25:RA:634:C:H2'   | 25:RA:635:C:C6    | 2.49                     | 0.47              |
| 25:RA:669:G:H2'   | 25:RA:669:G:N3    | 2.30                     | 0.47              |
| 25:RA:1264:G:H5'  | 51:R5:11:THR:CG2  | 2.42                     | 0.47              |
| 27:RD:72:LYS:CG   | 27:RD:103:ARG:NH2 | 2.77                     | 0.47              |
| 28:RE:54:GLN:N    | 28:RE:54:GLN:CD   | 2.73                     | 0.47              |
| 28:RE:56:PRO:O    | 28:RE:57:LYS:CB   | 2.61                     | 0.47              |
| 30:RG:13:GLU:O    | 30:RG:13:GLU:HG3  | 2.14                     | 0.47              |
| 30:RG:106:LEU:HA  | 30:RG:110:ALA:CB  | 2.44                     | 0.47              |
| 33:RN:4:TYR:OH    | 33:RN:7:LYS:NZ    | 2.46                     | 0.47              |
| 33:RN:118:LYS:O   | 33:RN:120:LEU:N   | 2.43                     | 0.47              |
| 35:RP:13:ASN:C    | 35:RP:15:ARG:H    | 2.21                     | 0.47              |
| 35:RP:19:VAL:CG2  | 35:RP:20:GLY:H    | 1.98                     | 0.47              |
| 36:RQ:66:ILE:H    | 36:RQ:104:PHE:HA  | 1.79                     | 0.47              |
| 38:RS:40:ILE:HG22 | 38:RS:41:ASP:N    | 2.28                     | 0.47              |
| 39:RT:96:ARG:NH1  | 39:RT:96:ARG:CB   | 2.77                     | 0.47              |
| 43:RX:6:ASP:OD1   | 48:R2:29:LYS:NZ   | 2.47                     | 0.47              |
| 44:RY:81:LYS:HZ2  | 44:RY:98:VAL:CG1  | 2.26                     | 0.47              |
| 48:R2:4:SER:OG    | 48:R2:5:GLU:OE2   | 2.26                     | 0.47              |
| 52:R6:8:LYS:O     | 52:R6:27:LYS:HG2  | 2.14                     | 0.47              |
| 1:XA:339:C:OP2    | 34:YO:97:ARG:NH1  | 2.48                     | 0.47              |
| 1:XA:730:G:C5     | 1:XA:731:G:H1'    | 2.50                     | 0.47              |
| 2:XB:109:SER:C    | 2:XB:111:ARG:H    | 2.21                     | 0.47              |
| 3:XC:12:LEU:C     | 3:XC:14:ILE:H     | 2.22                     | 0.47              |
| 3:XC:95:THR:CG2   | 3:XC:96:GLY:H     | 2.09                     | 0.47              |
| 4:XD:22:LYS:HD3   | 4:XD:26:CYS:SG    | 2.49                     | 0.47              |
| 4:XD:29:PRO:O     | 4:XD:30:LYS:HB3   | 2.15                     | 0.47              |
| 5:XE:82:VAL:CG1   | 5:XE:83:GLU:H     | 2.27                     | 0.47              |
| 5:XE:141:GLN:HA   | 5:XE:143:ARG:HH12 | 1.79                     | 0.47              |
| 8:XH:86:ILE:HG12  | 8:XH:135:CYS:HA   | 1.96                     | 0.47              |
| 10:XJ:49:VAL:HG23 | 14:YN:34:TYR:OH   | 2.13                     | 0.47              |
| 17:XQ:29:HIS:N    | 17:XQ:33:GLY:O    | 2.47                     | 0.47              |
| 19:XS:41:VAL:CB   | 19:XS:42:PRO:CA   | 2.76                     | 0.47              |
| 25:YA:674:G:N2    | 25:YA:2444:G:O3'  | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:784:A:N7     | 27:YD:229:VAL:HG21 | 2.29                     | 0.47              |
| 25:YA:1109:C:O2'   | 25:YA:1110:G:OP1   | 2.31                     | 0.47              |
| 25:YA:1365:A:OP2   | 47:Y1:3:LYS:HB2    | 2.14                     | 0.47              |
| 25:YA:2267:A:H5''  | 25:YA:2268:A:H5'   | 1.95                     | 0.47              |
| 25:YA:2563:U:H1'   | 25:YA:2566:A:N6    | 2.29                     | 0.47              |
| 25:YA:2788:C:O2'   | 25:YA:2809:A:N3    | 2.45                     | 0.47              |
| 27:YD:134:ARG:HB2  | 27:YD:135:PHE:CD2  | 2.49                     | 0.47              |
| 28:YE:36:ARG:HH11  | 28:YE:36:ARG:CB    | 2.28                     | 0.47              |
| 28:YE:65:GLY:HA2   | 28:YE:70:ALA:HB3   | 1.95                     | 0.47              |
| 28:YE:203:LYS:HD2  | 28:YE:203:LYS:C    | 2.39                     | 0.47              |
| 30:YG:12:TYR:O     | 30:YG:16:ARG:HB3   | 2.15                     | 0.47              |
| 31:YH:127:GLU:OE2  | 31:YH:130:ARG:NH2  | 2.47                     | 0.47              |
| 33:YN:9:VAL:HG21   | 33:YN:48:MET:CB    | 2.45                     | 0.47              |
| 33:YN:137:LYS:CG   | 33:YN:138:LEU:N    | 2.77                     | 0.47              |
| 35:YP:112:LEU:HD12 | 35:YP:127:ALA:CB   | 2.44                     | 0.47              |
| 37:YR:56:LYS:HE2   | 37:YR:94:TYR:OH    | 2.14                     | 0.47              |
| 39:YT:132:LYS:O    | 39:YT:136:GLN:HG3  | 2.13                     | 0.47              |
| 41:YV:59:ALA:HB2   | 41:YV:96:ILE:HD13  | 1.97                     | 0.47              |
| 44:YY:81:LYS:HZ2   | 44:YY:98:VAL:CG1   | 2.27                     | 0.47              |
| 48:Y2:17:SER:CB    | 48:Y2:18:PRO:CA    | 2.92                     | 0.47              |
| 51:Y5:48:GLU:HA    | 51:Y5:59:GLU:CG    | 2.43                     | 0.47              |
| 1:QA:210:U:O2'     | 1:QA:216:G:N7      | 2.43                     | 0.47              |
| 1:QA:532:A:H2      | 1:QA:1206:G:H21    | 1.61                     | 0.47              |
| 1:QA:701:C:O2      | 1:QA:703:G:N1      | 2.48                     | 0.47              |
| 1:QA:1145:C:O2'    | 1:QA:1146:A:N7     | 2.40                     | 0.47              |
| 2:QB:164:VAL:HB    | 2:QB:186:ALA:HB1   | 1.96                     | 0.47              |
| 3:QC:148:GLY:O     | 3:QC:202:ILE:HA    | 2.13                     | 0.47              |
| 4:QD:19:LEU:O      | 4:QD:20:TYR:C      | 2.57                     | 0.47              |
| 4:QD:198:VAL:CG1   | 4:QD:199:ASN:N     | 2.75                     | 0.47              |
| 5:QE:20:GLN:O      | 5:QE:21:ALA:C      | 2.57                     | 0.47              |
| 7:QG:79:ARG:HG2    | 7:QG:79:ARG:NH1    | 2.29                     | 0.47              |
| 8:QH:39:LEU:HD11   | 8:QH:111:ILE:HD11  | 1.96                     | 0.47              |
| 9:QI:118:LYS:HB3   | 9:QI:118:LYS:HZ3   | 1.80                     | 0.47              |
| 14:QN:12:ARG:C     | 14:QN:14:PRO:CD    | 2.81                     | 0.47              |
| 16:QP:40:ASP:C     | 16:QP:42:ARG:N     | 2.73                     | 0.47              |
| 18:QR:53:ARG:C     | 18:QR:55:ARG:H     | 2.22                     | 0.47              |
| 25:RA:1113:U:H2'   | 25:RA:1114:G:C8    | 2.49                     | 0.47              |
| 25:RA:1486:A:H2'   | 25:RA:1487:G:C8    | 2.49                     | 0.47              |
| 25:RA:1795:C:O2    | 27:RD:255:LYS:HE2  | 2.14                     | 0.47              |
| 25:RA:2198:A:C2    | 32:RI:29:TYR:HB2   | 2.49                     | 0.47              |
| 28:RE:3:GLY:HA3    | 28:RE:81:ILE:HG21  | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:N    | 2.29                     | 0.47              |
| 30:RG:5:VAL:HG22   | 50:R4:25:TYR:CE2   | 2.50                     | 0.47              |
| 31:RH:53:GLU:CD    | 31:RH:54:ARG:H     | 2.21                     | 0.47              |
| 33:RN:15:LEU:C     | 33:RN:15:LEU:HD13  | 2.40                     | 0.47              |
| 41:RV:21:ARG:HD2   | 41:RV:91:TYR:CZ    | 2.49                     | 0.47              |
| 41:RV:38:LEU:HD23  | 41:RV:39:LEU:H     | 1.79                     | 0.47              |
| 44:RY:19:LYS:HE3   | 44:RY:20:TYR:CE1   | 2.49                     | 0.47              |
| 44:RY:39:VAL:O     | 44:RY:40:GLU:OE2   | 2.32                     | 0.47              |
| 47:R1:94:LEU:O     | 47:R1:95:LEU:CB    | 2.62                     | 0.47              |
| 48:R2:6:VAL:O      | 48:R2:7:ARG:C      | 2.57                     | 0.47              |
| 50:R4:23:GLU:C     | 50:R4:24:THR:HG1   | 2.22                     | 0.47              |
| 1:XA:148:G:H1      | 1:XA:174:C:H42     | 1.63                     | 0.47              |
| 1:XA:222:U:H2'     | 1:XA:223:U:C6      | 2.49                     | 0.47              |
| 1:XA:779:C:H4'     | 11:XK:121:PRO:O    | 2.15                     | 0.47              |
| 2:XB:200:ILE:H     | 2:XB:200:ILE:HD12  | 1.79                     | 0.47              |
| 6:XF:97:PHE:CD2    | 18:XR:31:LEU:HD21  | 2.48                     | 0.47              |
| 8:XH:39:LEU:HD11   | 8:XH:111:ILE:HD11  | 1.96                     | 0.47              |
| 12:XL:43:VAL:HG23  | 12:XL:93:LEU:HD22  | 1.97                     | 0.47              |
| 16:XP:21:VAL:HG23  | 16:XP:34:GLU:H     | 1.79                     | 0.47              |
| 20:XT:49:ALA:HB2   | 20:XT:99:LEU:HD22  | 1.97                     | 0.47              |
| 20:XT:50:GLU:CG    | 20:XT:51:GLU:N     | 2.76                     | 0.47              |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:C8  | 2.50                     | 0.47              |
| 25:YA:529:A:H8     | 25:YA:530:G:C6     | 2.33                     | 0.47              |
| 25:YA:592:G:H1     | 25:YA:665:C:H42    | 1.62                     | 0.47              |
| 25:YA:1796:U:H2'   | 25:YA:1797:C:C6    | 2.50                     | 0.47              |
| 25:YA:1862:G:H2'   | 25:YA:1863:G:C8    | 2.47                     | 0.47              |
| 28:YE:56:PRO:O     | 28:YE:57:LYS:CB    | 2.61                     | 0.47              |
| 30:YG:88:ILE:O     | 30:YG:88:ILE:CD1   | 2.54                     | 0.47              |
| 31:YH:154:PRO:CG   | 31:YH:162:ILE:O    | 2.61                     | 0.47              |
| 33:YN:15:LEU:C     | 33:YN:15:LEU:HD13  | 2.39                     | 0.47              |
| 33:YN:67:LEU:O     | 33:YN:88:GLU:HG3   | 2.14                     | 0.47              |
| 35:YP:147:LEU:N    | 35:YP:147:LEU:HD22 | 2.29                     | 0.47              |
| 37:YR:1:MET:SD     | 37:YR:1:MET:N      | 2.75                     | 0.47              |
| 40:YU:92:ARG:CZ    | 40:YU:94:ASN:HD22  | 2.27                     | 0.47              |
| 48:Y2:6:VAL:O      | 48:Y2:7:ARG:C      | 2.57                     | 0.47              |
| 48:Y2:48:HIS:O     | 48:Y2:49:LYS:C     | 2.57                     | 0.47              |
| 1:QA:1024:G:H4'    | 1:QA:1024:G:OP1    | 2.14                     | 0.47              |
| 1:QA:1224:G:N1     | 1:QA:1322:C:H1'    | 2.29                     | 0.47              |
| 2:QB:92:TYR:C      | 2:QB:92:TYR:HD1    | 2.21                     | 0.47              |
| 4:QD:30:LYS:CD     | 4:QD:30:LYS:H      | 2.23                     | 0.47              |
| 9:QI:128:ARG:NH1   | 22:QV:33:U:OP2     | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:QL:50:SER:O     | 12:QL:51:ALA:HB2   | 2.14                     | 0.47              |
| 22:QV:76:A:H2'     | 25:RA:2602:A:H61   | 1.77                     | 0.47              |
| 25:RA:27:G:HO2'    | 25:RA:28:A:H8      | 1.62                     | 0.47              |
| 25:RA:247:G:H4'    | 25:RA:386:G:C5     | 2.49                     | 0.47              |
| 25:RA:389:G:N1     | 35:RP:70:GLN:HB3   | 2.30                     | 0.47              |
| 25:RA:1509:C:H2'   | 25:RA:1511:A:C8    | 2.50                     | 0.47              |
| 25:RA:2638:G:OP2   | 28:RE:82:ARG:NH2   | 2.48                     | 0.47              |
| 26:RB:3:C:H2'      | 26:RB:4:C:H6       | 1.79                     | 0.47              |
| 27:RD:177:LEU:C    | 27:RD:179:SER:H    | 2.23                     | 0.47              |
| 29:RF:162:LEU:HD23 | 29:RF:165:ARG:HH21 | 1.80                     | 0.47              |
| 33:RN:137:LYS:CG   | 33:RN:138:LEU:H    | 2.27                     | 0.47              |
| 35:RP:147:LEU:N    | 35:RP:147:LEU:HD22 | 2.29                     | 0.47              |
| 37:RR:117:VAL:O    | 37:RR:118:GLU:CB   | 2.62                     | 0.47              |
| 38:RS:95:HIS:O     | 38:RS:96:GLY:C     | 2.57                     | 0.47              |
| 38:RS:108:GLY:O    | 38:RS:110:LEU:N    | 2.48                     | 0.47              |
| 52:R6:33:LYS:C     | 52:R6:35:GLU:H     | 2.22                     | 0.47              |
| 55:R9:1:MET:SD     | 55:R9:31:LYS:O     | 2.73                     | 0.47              |
| 1:XA:271:C:H2'     | 1:XA:272:C:C6      | 2.50                     | 0.47              |
| 1:XA:1129:C:C4'    | 1:XA:1130:A:H5'    | 2.41                     | 0.47              |
| 1:XA:1222:G:H5''   | 19:XS:78:ARG:NH1   | 2.30                     | 0.47              |
| 1:XA:1446:A:HO2'   | 1:XA:1447:G:P      | 2.36                     | 0.47              |
| 2:XB:172:ILE:O     | 2:XB:175:ARG:CB    | 2.63                     | 0.47              |
| 2:XB:204:ASN:HD22  | 2:XB:204:ASN:C     | 2.22                     | 0.47              |
| 4:XD:150:GLU:C     | 4:XD:152:SER:N     | 2.73                     | 0.47              |
| 6:XF:40:VAL:HG22   | 6:XF:41:GLU:N      | 2.30                     | 0.47              |
| 7:XG:50:ILE:HG21   | 7:XG:61:VAL:HG21   | 1.97                     | 0.47              |
| 7:XG:78:ARG:HG3    | 7:XG:78:ARG:HH11   | 1.78                     | 0.47              |
| 9:XI:18:PHE:HB2    | 9:XI:62:TYR:HB3    | 1.95                     | 0.47              |
| 9:XI:80:GLY:C      | 9:XI:82:ALA:N      | 2.70                     | 0.47              |
| 11:XK:32:ILE:HD11  | 11:XK:68:ALA:O     | 2.14                     | 0.47              |
| 16:XP:40:ASP:C     | 16:XP:42:ARG:N     | 2.73                     | 0.47              |
| 25:YA:26:G:C6      | 25:YA:27:G:C2      | 3.02                     | 0.47              |
| 25:YA:563:G:H22    | 25:YA:578:A:H2     | 1.61                     | 0.47              |
| 25:YA:1336:A:H2'   | 25:YA:1337:G:C8    | 2.50                     | 0.47              |
| 25:YA:1972:A:H2'   | 25:YA:1973:G:H8    | 1.79                     | 0.47              |
| 25:YA:2336:A:H61   | 46:Y0:43:THR:CG2   | 2.27                     | 0.47              |
| 26:YB:15:A:H5'     | 26:YB:16:G:H8      | 1.73                     | 0.47              |
| 28:YE:52:LEU:HB2   | 28:YE:75:VAL:CG2   | 2.40                     | 0.47              |
| 30:YG:5:VAL:HG22   | 50:Y4:25:TYR:CE2   | 2.50                     | 0.47              |
| 30:YG:106:LEU:HA   | 30:YG:110:ALA:CB   | 2.44                     | 0.47              |
| 32:YI:62:LYS:HE3   | 32:YI:134:PRO:HG2  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:YP:126:VAL:HA  | 35:YP:145:PRO:HD2 | 1.95                     | 0.47              |
| 39:YT:29:ARG:NH1  | 39:YT:46:GLU:OE1  | 2.48                     | 0.47              |
| 40:YU:106:PHE:O   | 40:YU:109:LEU:HB2 | 2.15                     | 0.47              |
| 42:YW:81:ALA:C    | 42:YW:82:LEU:HD12 | 2.40                     | 0.47              |
| 43:YX:35:THR:O    | 43:YX:37:THR:N    | 2.47                     | 0.47              |
| 50:Y4:50:VAL:O    | 50:Y4:50:VAL:CG1  | 2.62                     | 0.47              |
| 52:Y6:33:LYS:C    | 52:Y6:35:GLU:H    | 2.22                     | 0.47              |
| 1:QA:109:A:C6     | 1:QA:326:G:C6     | 3.02                     | 0.47              |
| 1:QA:182:U:C4     | 1:QA:183:G:H1'    | 2.50                     | 0.47              |
| 1:QA:792:A:H4'    | 1:QA:793:U:O5'    | 2.14                     | 0.47              |
| 1:QA:1002:G:H2'   | 1:QA:1003:G:C8    | 2.49                     | 0.47              |
| 1:QA:1065:U:O2'   | 1:QA:1066:C:OP2   | 2.26                     | 0.47              |
| 1:QA:1291:G:H4'   | 9:QI:39:GLY:HA3   | 1.96                     | 0.47              |
| 2:QB:69:LEU:HB3   | 2:QB:162:ILE:HG22 | 1.95                     | 0.47              |
| 2:QB:223:ILE:HA   | 2:QB:226:ARG:HB3  | 1.97                     | 0.47              |
| 3:QC:113:ALA:C    | 3:QC:115:LEU:N    | 2.73                     | 0.47              |
| 3:QC:203:PHE:O    | 3:QC:204:LEU:HD23 | 2.14                     | 0.47              |
| 4:QD:154:ASN:O    | 4:QD:155:LEU:O    | 2.32                     | 0.47              |
| 6:QF:79:LEU:O     | 6:QF:85:VAL:HG11  | 2.14                     | 0.47              |
| 8:QH:80:ILE:HG23  | 8:QH:137:VAL:HG12 | 1.97                     | 0.47              |
| 8:QH:82:HIS:CD2   | 8:QH:83:ILE:N     | 2.82                     | 0.47              |
| 8:QH:86:ILE:HG22  | 8:QH:87:SER:N     | 2.29                     | 0.47              |
| 10:QJ:40:LEU:HB2  | 10:QJ:69:ASN:CB   | 2.40                     | 0.47              |
| 10:QJ:74:ILE:HG12 | 10:QJ:74:ILE:O    | 2.13                     | 0.47              |
| 11:QK:32:ILE:HD11 | 11:QK:68:ALA:O    | 2.14                     | 0.47              |
| 11:QK:91:ARG:HH22 | 18:QR:88:LYS:HZ3  | 1.61                     | 0.47              |
| 12:QL:11:VAL:HG21 | 17:QQ:34:LYS:HD3  | 1.96                     | 0.47              |
| 13:QM:72:ALA:O    | 13:QM:76:ALA:HB2  | 2.14                     | 0.47              |
| 14:QN:41:ARG:CG   | 14:QN:41:ARG:HH11 | 2.28                     | 0.47              |
| 14:QN:47:LEU:O    | 14:QN:48:ALA:C    | 2.57                     | 0.47              |
| 16:QP:34:GLU:HG2  | 16:QP:35:LYS:N    | 2.29                     | 0.47              |
| 17:QQ:76:LEU:HD11 | 17:QQ:79:SER:H    | 1.80                     | 0.47              |
| 18:QR:32:ARG:HH11 | 18:QR:65:ILE:HD13 | 1.80                     | 0.47              |
| 18:QR:82:THR:HG22 | 18:QR:83:GLU:H    | 1.79                     | 0.47              |
| 19:QS:68:GLY:HA3  | 50:R4:68:ARG:CB   | 2.45                     | 0.47              |
| 25:RA:31:C:O2'    | 25:RA:1238:G:H5'  | 2.15                     | 0.47              |
| 25:RA:180:G:N1    | 25:RA:214:G:O6    | 2.47                     | 0.47              |
| 25:RA:528:A:H2    | 25:RA:2043:C:O5'  | 1.98                     | 0.47              |
| 25:RA:1019:U:O2'  | 25:RA:1021:A:H2   | 1.98                     | 0.47              |
| 25:RA:1153:C:H2'  | 25:RA:1154:G:O4'  | 2.15                     | 0.47              |
| 25:RA:1486:A:H2'  | 25:RA:1487:G:H8   | 1.79                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2122:U:H2'  | 25:RA:2123:G:C8    | 2.48                     | 0.47              |
| 25:RA:2257:U:H2'  | 25:RA:2258:C:C6    | 2.49                     | 0.47              |
| 25:RA:2415:G:H4'  | 35:RP:66:GLY:C     | 2.39                     | 0.47              |
| 25:RA:2722:G:H4'  | 37:RR:4:LEU:HB2    | 1.96                     | 0.47              |
| 25:RA:2836:U:H2'  | 25:RA:2837:G:C8    | 2.50                     | 0.47              |
| 28:RE:65:GLY:HA2  | 28:RE:70:ALA:HB3   | 1.95                     | 0.47              |
| 28:RE:101:ARG:C   | 28:RE:201:THR:OG1  | 2.58                     | 0.47              |
| 28:RE:197:ILE:CD1 | 28:RE:199:ARG:HH12 | 2.26                     | 0.47              |
| 29:RF:184:TYR:CD2 | 29:RF:188:ARG:HD2  | 2.50                     | 0.47              |
| 30:RG:56:ALA:HB2  | 30:RG:153:ARG:NE   | 2.28                     | 0.47              |
| 30:RG:109:VAL:C   | 30:RG:112:PRO:HD2  | 2.40                     | 0.47              |
| 31:RH:126:PRO:CG  | 31:RH:127:GLU:N    | 2.65                     | 0.47              |
| 33:RN:57:ALA:CA   | 33:RN:60:ILE:HD11  | 2.44                     | 0.47              |
| 34:RO:37:ASP:O    | 34:RO:62:VAL:HG23  | 2.15                     | 0.47              |
| 34:RO:120:GLU:OE1 | 39:RT:67:SER:OG    | 2.25                     | 0.47              |
| 35:RP:37:GLY:O    | 35:RP:41:ARG:HD3   | 2.15                     | 0.47              |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:CB   | 2.35                     | 0.47              |
| 36:RQ:86:GLY:O    | 36:RQ:88:GLY:N     | 2.46                     | 0.47              |
| 37:RR:74:LYS:O    | 37:RR:76:VAL:N     | 2.45                     | 0.47              |
| 41:RV:36:PRO:HA   | 41:RV:56:SER:CB    | 2.44                     | 0.47              |
| 42:RW:28:SER:C    | 42:RW:30:GLU:N     | 2.70                     | 0.47              |
| 44:RY:61:ILE:HG22 | 44:RY:62:GLU:N     | 2.28                     | 0.47              |
| 50:R4:8:LYS:O     | 50:R4:9:LEU:CB     | 2.62                     | 0.47              |
| 51:R5:39:MET:C    | 51:R5:40:LYS:HG3   | 2.39                     | 0.47              |
| 52:R6:20:ASN:ND2  | 52:R6:42:TRP:CZ2   | 2.82                     | 0.47              |
| 54:R8:44:LYS:HD2  | 54:R8:44:LYS:N     | 2.30                     | 0.47              |
| 55:R9:19:ARG:NH2  | 55:R9:26:ILE:HD11  | 2.29                     | 0.47              |
| 1:XA:1297:C:O2'   | 1:XA:1298:C:P      | 2.72                     | 0.47              |
| 1:XA:1312:G:P     | 50:Y4:58:ARG:HH12  | 2.38                     | 0.47              |
| 2:XB:60:ASP:C     | 2:XB:62:ALA:N      | 2.71                     | 0.47              |
| 2:XB:71:VAL:HG23  | 2:XB:164:VAL:HG13  | 1.97                     | 0.47              |
| 2:XB:92:TYR:C     | 2:XB:92:TYR:HD1    | 2.22                     | 0.47              |
| 2:XB:168:THR:CB   | 2:XB:192:SER:HB2   | 2.41                     | 0.47              |
| 2:XB:220:ASP:O    | 2:XB:223:ILE:N     | 2.48                     | 0.47              |
| 2:XB:224:GLN:HA   | 2:XB:229:VAL:HG23  | 1.97                     | 0.47              |
| 3:XC:16:ARG:NH2   | 3:XC:183:ASP:OD2   | 2.48                     | 0.47              |
| 3:XC:52:LEU:H     | 3:XC:52:LEU:CD2    | 2.20                     | 0.47              |
| 3:XC:127:ARG:CG   | 3:XC:127:ARG:NH1   | 2.74                     | 0.47              |
| 3:XC:203:PHE:O    | 3:XC:204:LEU:HD23  | 2.14                     | 0.47              |
| 4:XD:94:LEU:HD12  | 4:XD:94:LEU:N      | 2.13                     | 0.47              |
| 4:XD:114:ARG:NH1  | 4:XD:114:ARG:CG    | 2.77                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:XD:153:ARG:CZ    | 4:XD:181:MET:HG3  | 2.44                     | 0.47              |
| 5:XE:13:ILE:HG22   | 5:XE:13:ILE:O     | 2.14                     | 0.47              |
| 5:XE:63:ARG:C      | 5:XE:66:MET:HE2   | 2.39                     | 0.47              |
| 6:XF:40:VAL:HG22   | 6:XF:41:GLU:H     | 1.80                     | 0.47              |
| 7:XG:92:SER:HB3    | 7:XG:95:ARG:CB    | 2.45                     | 0.47              |
| 8:XH:6:ILE:O       | 8:XH:10:LEU:HG    | 2.14                     | 0.47              |
| 8:XH:10:LEU:H      | 8:XH:10:LEU:CD2   | 2.15                     | 0.47              |
| 9:XI:106:ALA:O     | 9:XI:108:VAL:HG13 | 2.15                     | 0.47              |
| 11:XK:32:ILE:HD12  | 11:XK:72:ALA:CB   | 2.36                     | 0.47              |
| 13:XM:8:GLU:OE2    | 30:YG:115:ARG:CZ  | 2.62                     | 0.47              |
| 13:XM:8:GLU:CD     | 30:YG:115:ARG:CZ  | 2.88                     | 0.47              |
| 13:XM:23:TYR:HB2   | 13:XM:67:GLU:OE1  | 2.15                     | 0.47              |
| 14:XN:41:ARG:NE    | 14:XN:42:ILE:HG13 | 2.29                     | 0.47              |
| 15:XO:76:GLU:O     | 15:XO:78:TYR:N    | 2.48                     | 0.47              |
| 17:XQ:63:ARG:HG2   | 17:XQ:64:PRO:CD   | 2.45                     | 0.47              |
| 17:XQ:82:MET:C     | 17:XQ:84:LEU:N    | 2.72                     | 0.47              |
| 25:YA:479:A:N3     | 25:YA:481:G:H5''  | 2.29                     | 0.47              |
| 25:YA:550:G:O2'    | 25:YA:1220:A:N3   | 2.40                     | 0.47              |
| 25:YA:559:G:H22    | 40:YU:49:HIS:CE1  | 2.32                     | 0.47              |
| 25:YA:570:G:H22    | 25:YA:2498:C:H4'  | 1.79                     | 0.47              |
| 25:YA:651:G:H5'    | 54:Y8:18:ALA:HB3  | 1.95                     | 0.47              |
| 25:YA:749:C:O2     | 25:YA:1618:A:H2'  | 2.15                     | 0.47              |
| 25:YA:1384:A:N3    | 25:YA:1405:U:H1'  | 2.29                     | 0.47              |
| 25:YA:1394:U:C4    | 25:YA:1395:A:C6   | 3.02                     | 0.47              |
| 25:YA:1826:G:H4'   | 27:YD:242:ARG:NH2 | 2.25                     | 0.47              |
| 25:YA:2291:U:H2'   | 25:YA:2292:C:C6   | 2.50                     | 0.47              |
| 25:YA:2761:G:H1'   | 31:YH:143:GLN:OE1 | 2.15                     | 0.47              |
| 27:YD:32:SER:O     | 27:YD:33:LEU:CB   | 2.60                     | 0.47              |
| 27:YD:35:LYS:HD3   | 27:YD:63:ARG:HB3  | 1.96                     | 0.47              |
| 27:YD:177:LEU:C    | 27:YD:179:SER:H   | 2.23                     | 0.47              |
| 28:YE:22:PRO:O     | 28:YE:22:PRO:CG   | 2.63                     | 0.47              |
| 28:YE:78:LEU:CD2   | 28:YE:79:ARG:HD2  | 2.43                     | 0.47              |
| 28:YE:89:ASP:O     | 28:YE:90:THR:O    | 2.33                     | 0.47              |
| 30:YG:14:GLU:O     | 30:YG:17:PRO:HG2  | 2.15                     | 0.47              |
| 30:YG:16:ARG:NH2   | 30:YG:28:VAL:O    | 2.48                     | 0.47              |
| 31:YH:131:VAL:HG12 | 31:YH:132:ARG:N   | 2.29                     | 0.47              |
| 33:YN:42:TRP:HA    | 33:YN:48:MET:CE   | 2.42                     | 0.47              |
| 33:YN:57:ALA:CA    | 33:YN:60:ILE:HD11 | 2.44                     | 0.47              |
| 33:YN:73:THR:HA    | 33:YN:83:LYS:O    | 2.15                     | 0.47              |
| 35:YP:81:GLN:HB3   | 35:YP:110:TYR:HB3 | 1.97                     | 0.47              |
| 35:YP:98:GLU:O     | 35:YP:99:LEU:C    | 2.57                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:59:ARG:CD   | 36:YQ:59:ARG:N    | 2.73                     | 0.47              |
| 36:YQ:80:GLU:HG3  | 36:YQ:81:VAL:N    | 2.27                     | 0.47              |
| 38:YS:46:VAL:HG12 | 38:YS:47:THR:N    | 2.28                     | 0.47              |
| 38:YS:95:HIS:O    | 38:YS:96:GLY:C    | 2.57                     | 0.47              |
| 39:YT:3:ARG:O     | 39:YT:4:GLY:C     | 2.58                     | 0.47              |
| 39:YT:51:ARG:CG   | 39:YT:98:LYS:HG3  | 2.44                     | 0.47              |
| 42:YW:66:GLU:O    | 42:YW:69:LEU:HG   | 2.14                     | 0.47              |
| 43:YX:43:VAL:HG11 | 43:YX:51:VAL:HG21 | 1.97                     | 0.47              |
| 44:YY:19:LYS:HE3  | 44:YY:20:TYR:CE1  | 2.49                     | 0.47              |
| 50:Y4:33:VAL:CG1  | 50:Y4:34:GLU:H    | 2.22                     | 0.47              |
| 50:Y4:50:VAL:O    | 50:Y4:50:VAL:HG13 | 2.15                     | 0.47              |
| 1:QA:97:U:H2'     | 1:QA:99:C:C6      | 2.50                     | 0.47              |
| 1:QA:428:G:O3'    | 4:QD:36:ARG:NH2   | 2.47                     | 0.47              |
| 1:QA:1306:A:C6    | 1:QA:1307:U:C2    | 3.03                     | 0.47              |
| 2:QB:60:ASP:C     | 2:QB:62:ALA:N     | 2.72                     | 0.47              |
| 2:QB:71:VAL:HG23  | 2:QB:164:VAL:HG13 | 1.97                     | 0.47              |
| 2:QB:95:GLN:NE2   | 2:QB:147:LYS:HE2  | 2.27                     | 0.47              |
| 2:QB:220:ASP:O    | 2:QB:223:ILE:N    | 2.48                     | 0.47              |
| 3:QC:11:ARG:HG2   | 3:QC:11:ARG:HH11  | 1.80                     | 0.47              |
| 5:QE:101:ILE:CD1  | 5:QE:119:LEU:HD23 | 2.36                     | 0.47              |
| 7:QG:70:LYS:O     | 7:QG:138:LYS:HE3  | 2.15                     | 0.47              |
| 13:QM:23:TYR:HB3  | 13:QM:67:GLU:CG   | 2.39                     | 0.47              |
| 16:QP:69:THR:O    | 16:QP:73:LEU:HG   | 2.14                     | 0.47              |
| 17:QQ:63:ARG:HG2  | 17:QQ:64:PRO:CD   | 2.45                     | 0.47              |
| 18:QR:64:ARG:O    | 18:QR:65:ILE:C    | 2.58                     | 0.47              |
| 19:QS:11:VAL:O    | 19:QS:12:ASP:CB   | 2.61                     | 0.47              |
| 21:QU:15:ARG:HG2  | 21:QU:15:ARG:NH1  | 2.29                     | 0.47              |
| 25:RA:153:C:OP2   | 47:R1:88:LYS:HE2  | 2.15                     | 0.47              |
| 25:RA:482:A:H4'   | 44:RY:47:LYS:HD2  | 1.97                     | 0.47              |
| 25:RA:769:G:H5'   | 25:RA:1379:A:H61  | 1.79                     | 0.47              |
| 25:RA:2638:G:P    | 28:RE:82:ARG:HH22 | 2.37                     | 0.47              |
| 28:RE:17:ASP:N    | 28:RE:17:ASP:OD2  | 2.46                     | 0.47              |
| 28:RE:63:LEU:O    | 28:RE:64:LYS:CB   | 2.62                     | 0.47              |
| 28:RE:121:ASN:O   | 28:RE:122:PHE:C   | 2.57                     | 0.47              |
| 34:RO:53:LYS:CD   | 34:RO:56:ASP:OD1  | 2.63                     | 0.47              |
| 42:RW:81:ALA:C    | 42:RW:82:LEU:HD12 | 2.40                     | 0.47              |
| 50:R4:3:GLU:HG3   | 50:R4:4:GLY:H     | 1.79                     | 0.47              |
| 1:XA:439:A:OP2    | 1:XA:493:G:N1     | 2.48                     | 0.47              |
| 1:XA:606:G:N2     | 1:XA:631:G:H8     | 2.12                     | 0.47              |
| 1:XA:1024:G:OP1   | 1:XA:1024:G:H4'   | 2.15                     | 0.47              |
| 1:XA:1206:G:H4'   | 3:XC:192:THR:O    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1225:A:H5''  | 1:XA:1226:C:OP2   | 2.15                     | 0.47              |
| 2:XB:116:GLU:HA   | 2:XB:119:GLU:HB3  | 1.96                     | 0.47              |
| 2:XB:158:LEU:HD12 | 2:XB:158:LEU:C    | 2.38                     | 0.47              |
| 2:XB:223:ILE:HA   | 2:XB:226:ARG:HB3  | 1.97                     | 0.47              |
| 3:XC:8:ILE:C      | 3:XC:10:PHE:N     | 2.69                     | 0.47              |
| 3:XC:143:GLU:C    | 3:XC:145:GLY:H    | 2.23                     | 0.47              |
| 4:XD:19:LEU:O     | 4:XD:20:TYR:C     | 2.58                     | 0.47              |
| 4:XD:126:ILE:HG22 | 4:XD:127:THR:H    | 1.80                     | 0.47              |
| 6:XF:9:VAL:HB     | 6:XF:87:ARG:HB2   | 1.97                     | 0.47              |
| 7:XG:50:ILE:CG2   | 7:XG:61:VAL:HG21  | 2.45                     | 0.47              |
| 7:XG:51:GLN:OE1   | 7:XG:51:GLN:HA    | 2.14                     | 0.47              |
| 8:XH:82:HIS:CD2   | 8:XH:83:ILE:N     | 2.82                     | 0.47              |
| 11:XK:33:THR:HB   | 11:XK:37:GLY:C    | 2.40                     | 0.47              |
| 13:XM:28:ALA:C    | 13:XM:30:ALA:N    | 2.70                     | 0.47              |
| 18:XR:31:LEU:H    | 18:XR:31:LEU:CD2  | 2.27                     | 0.47              |
| 20:XT:93:GLU:HG2  | 20:XT:93:GLU:O    | 2.14                     | 0.47              |
| 25:YA:27:G:H22    | 25:YA:512:G:H2'   | 1.79                     | 0.47              |
| 25:YA:747:U:C4    | 25:YA:2613:U:C4   | 3.02                     | 0.47              |
| 25:YA:1262:A:N3   | 51:Y5:10:LYS:HE3  | 2.30                     | 0.47              |
| 25:YA:1636:C:H2'  | 25:YA:1637:A:C8   | 2.49                     | 0.47              |
| 25:YA:2243:U:H2'  | 25:YA:2244:U:C6   | 2.50                     | 0.47              |
| 25:YA:2660:A:H2'  | 25:YA:2661:G:O4'  | 2.14                     | 0.47              |
| 25:YA:2688:U:H1'  | 25:YA:2721:A:N6   | 2.29                     | 0.47              |
| 27:YD:31:LYS:C    | 27:YD:32:SER:O    | 2.54                     | 0.47              |
| 27:YD:72:LYS:CG   | 27:YD:103:ARG:NH2 | 2.77                     | 0.47              |
| 28:YE:54:GLN:N    | 28:YE:54:GLN:CD   | 2.73                     | 0.47              |
| 28:YE:103:ASP:OD2 | 28:YE:168:MET:HG2 | 2.15                     | 0.47              |
| 30:YG:106:LEU:HA  | 30:YG:110:ALA:HB3 | 1.95                     | 0.47              |
| 31:YH:67:LEU:O    | 31:YH:71:LEU:HB2  | 2.15                     | 0.47              |
| 34:YO:37:ASP:O    | 34:YO:62:VAL:HG23 | 2.14                     | 0.47              |
| 34:YO:104:ARG:HD3 | 39:YT:36:GLU:OE2  | 2.15                     | 0.47              |
| 35:YP:125:VAL:C   | 35:YP:145:PRO:HD2 | 2.39                     | 0.47              |
| 40:YU:66:ASN:CB   | 40:YU:76:TYR:HB2  | 2.44                     | 0.47              |
| 40:YU:104:GLN:CD  | 40:YU:104:GLN:H   | 2.16                     | 0.47              |
| 40:YU:107:ALA:O   | 40:YU:110:VAL:HB  | 2.14                     | 0.47              |
| 41:YV:4:ILE:HA    | 41:YV:12:TYR:O    | 2.14                     | 0.47              |
| 43:YX:87:GLN:C    | 43:YX:88:LYS:HG3  | 2.40                     | 0.47              |
| 44:YY:39:VAL:O    | 44:YY:40:GLU:OE2  | 2.32                     | 0.47              |
| 44:YY:56:PRO:O    | 44:YY:58:GLY:N    | 2.47                     | 0.47              |
| 47:Y1:83:GLU:OE1  | 47:Y1:85:LEU:HB2  | 2.15                     | 0.47              |
| 1:QA:1118:C:H5'   | 9:QI:104:ARG:HD3  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1162:C:H2'   | 1:QA:1163:C:O4'    | 2.15                     | 0.47              |
| 1:QA:1222:G:OP1   | 19:QS:77:THR:HG21  | 2.14                     | 0.47              |
| 1:QA:1224:G:H1    | 1:QA:1362(A):C:H42 | 1.62                     | 0.47              |
| 2:QB:5:ILE:O      | 2:QB:6:THR:O       | 2.32                     | 0.47              |
| 2:QB:158:LEU:HD12 | 2:QB:158:LEU:C     | 2.39                     | 0.47              |
| 2:QB:168:THR:CB   | 2:QB:192:SER:HB2   | 2.41                     | 0.47              |
| 3:QC:23:TYR:CG    | 3:QC:24:ALA:N      | 2.83                     | 0.47              |
| 3:QC:58:GLU:O     | 3:QC:59:ARG:HG3    | 2.15                     | 0.47              |
| 3:QC:195:VAL:CG1  | 3:QC:196:LEU:H     | 2.27                     | 0.47              |
| 4:QD:7:PRO:O      | 4:QD:10:ARG:HG2    | 2.15                     | 0.47              |
| 4:QD:9:CYS:SG     | 4:QD:22:LYS:HE3    | 2.55                     | 0.47              |
| 6:QF:40:VAL:HG22  | 6:QF:41:GLU:N      | 2.30                     | 0.47              |
| 11:QK:104:GLN:O   | 11:QK:106:LYS:HG3  | 2.15                     | 0.47              |
| 17:QQ:59:ILE:N    | 17:QQ:59:ILE:CD1   | 2.78                     | 0.47              |
| 20:QT:101:GLY:C   | 20:QT:103:GLY:N    | 2.73                     | 0.47              |
| 21:QU:14:TRP:CE3  | 21:QU:15:ARG:NH1   | 2.83                     | 0.47              |
| 25:RA:389:G:H22   | 35:RP:72:PRO:HD3   | 1.80                     | 0.47              |
| 25:RA:587:C:OP2   | 35:RP:21:ARG:NH2   | 2.48                     | 0.47              |
| 25:RA:1991:U:H2'  | 25:RA:1992:G:H5''  | 1.97                     | 0.47              |
| 25:RA:2625:G:H2'  | 25:RA:2626:C:O4'   | 2.15                     | 0.47              |
| 27:RD:102:LYS:O   | 27:RD:103:ARG:HG3  | 2.15                     | 0.47              |
| 29:RF:29:ASN:H    | 29:RF:112:MET:HE3  | 1.75                     | 0.47              |
| 33:RN:134:ARG:N   | 33:RN:135:PRO:CD   | 2.58                     | 0.47              |
| 35:RP:98:GLU:O    | 35:RP:99:LEU:C     | 2.57                     | 0.47              |
| 39:RT:3:ARG:O     | 39:RT:4:GLY:C      | 2.58                     | 0.47              |
| 42:RW:14:PRO:O    | 42:RW:15:ARG:C     | 2.58                     | 0.47              |
| 43:RX:26:TYR:HB3  | 43:RX:92:LEU:HD12  | 1.97                     | 0.47              |
| 43:RX:54:VAL:C    | 43:RX:55:ASN:HD22  | 2.23                     | 0.47              |
| 45:RZ:27:VAL:HG13 | 45:RZ:87:ASP:HB3   | 1.97                     | 0.47              |
| 45:RZ:28:MET:HE1  | 45:RZ:61:LEU:HD11  | 1.97                     | 0.47              |
| 48:R2:17:SER:CB   | 48:R2:18:PRO:CA    | 2.92                     | 0.47              |
| 1:XA:20:U:H1'     | 1:XA:916:G:N2      | 2.29                     | 0.47              |
| 1:XA:165:C:H2'    | 1:XA:166:G:C8      | 2.50                     | 0.47              |
| 1:XA:438:G:H4'    | 4:XD:123:HIS:CE1   | 2.50                     | 0.47              |
| 1:XA:720:C:H5''   | 18:XR:52:PRO:HA    | 1.97                     | 0.47              |
| 1:XA:1404:C:H2'   | 1:XA:1405:G:C8     | 2.50                     | 0.47              |
| 2:XB:33:TYR:C     | 2:XB:33:TYR:HD1    | 2.23                     | 0.47              |
| 2:XB:67:THR:C     | 2:XB:68:ILE:HD12   | 2.40                     | 0.47              |
| 5:XE:77:PRO:HG2   | 5:XE:142:LEU:HD22  | 1.97                     | 0.47              |
| 7:XG:70:LYS:O     | 7:XG:138:LYS:HE3   | 2.15                     | 0.47              |
| 9:XI:100:GLY:C    | 9:XI:102:LEU:N     | 2.71                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:YN:12:ARG:C     | 14:YN:14:PRO:CD    | 2.80                     | 0.47              |
| 18:XR:46:GLU:HG3   | 18:XR:47:THR:N     | 2.29                     | 0.47              |
| 25:YA:670:A:H5'    | 35:YP:43:GLY:HA2   | 1.97                     | 0.47              |
| 25:YA:752:A:H4'    | 25:YA:753:C:O5'    | 2.15                     | 0.47              |
| 25:YA:1045:A:N3    | 25:YA:1047:G:N2    | 2.62                     | 0.47              |
| 25:YA:1681:G:O2'   | 25:YA:1762:A:O2'   | 2.09                     | 0.47              |
| 25:YA:2096:U:H3    | 25:YA:2193:G:H1    | 1.62                     | 0.47              |
| 25:YA:2306:C:H2'   | 25:YA:2307:G:N2    | 2.26                     | 0.47              |
| 25:YA:2881:C:H2'   | 25:YA:2882:A:H8    | 1.79                     | 0.47              |
| 27:YD:231:HIS:ND1  | 27:YD:232:PRO:HD2  | 2.30                     | 0.47              |
| 29:YF:109:GLY:O    | 29:YF:110:LEU:C    | 2.58                     | 0.47              |
| 29:YF:127:GLU:OE1  | 29:YF:127:GLU:HA   | 2.07                     | 0.47              |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:HH21 | 1.79                     | 0.47              |
| 30:YG:109:VAL:C    | 30:YG:112:PRO:HD2  | 2.40                     | 0.47              |
| 31:YH:18:GLU:HA    | 31:YH:18:GLU:OE2   | 2.15                     | 0.47              |
| 33:YN:96:GLU:O     | 33:YN:97:ARG:C     | 2.57                     | 0.47              |
| 34:YO:53:LYS:CD    | 34:YO:56:ASP:OD1   | 2.63                     | 0.47              |
| 35:YP:115:LEU:CD1  | 35:YP:116:GLY:N    | 2.78                     | 0.47              |
| 37:YR:61:HIS:O     | 37:YR:65:LEU:HD13  | 2.14                     | 0.47              |
| 38:YS:99:LYS:C     | 38:YS:101:LEU:N    | 2.72                     | 0.47              |
| 42:YW:4:LYS:HA     | 42:YW:106:ILE:HA   | 1.97                     | 0.47              |
| 44:YY:44:ILE:O     | 44:YY:62:GLU:O     | 2.32                     | 0.47              |
| 51:Y5:57:VAL:O     | 51:Y5:57:VAL:HG13  | 2.14                     | 0.47              |
| 52:Y6:8:LYS:O      | 52:Y6:27:LYS:HG2   | 2.14                     | 0.47              |
| 52:Y6:20:ASN:O     | 52:Y6:21:TYR:HB2   | 2.15                     | 0.47              |
| 1:QA:643:C:H5'     | 8:QH:31:PHE:CE1    | 2.50                     | 0.47              |
| 1:QA:826:C:H2'     | 1:QA:827:U:O2      | 2.16                     | 0.47              |
| 1:QA:922:G:O2'     | 1:QA:1398:A:N1     | 2.35                     | 0.47              |
| 2:QB:172:ILE:O     | 2:QB:175:ARG:CB    | 2.62                     | 0.47              |
| 2:QB:204:ASN:HD22  | 2:QB:204:ASN:C     | 2.22                     | 0.47              |
| 4:QD:110:PHE:HD1   | 4:QD:110:PHE:H     | 1.63                     | 0.47              |
| 4:QD:146:ILE:HG22  | 4:QD:146:ILE:O     | 2.15                     | 0.47              |
| 6:QF:41:GLU:HG2    | 6:QF:43:LEU:CD1    | 2.44                     | 0.47              |
| 9:QI:106:ALA:O     | 9:QI:108:VAL:HG13  | 2.15                     | 0.47              |
| 11:QK:33:THR:HB    | 11:QK:37:GLY:C     | 2.40                     | 0.47              |
| 15:QO:76:GLU:O     | 15:QO:78:TYR:N     | 2.48                     | 0.47              |
| 17:QQ:82:MET:C     | 17:QQ:84:LEU:N     | 2.72                     | 0.47              |
| 25:RA:868:U:H2'    | 25:RA:869:G:O4'    | 2.15                     | 0.47              |
| 25:RA:1327:C:O3'   | 37:RR:105:ARG:NH2  | 2.48                     | 0.47              |
| 25:RA:1796:U:H2'   | 25:RA:1797:C:C6    | 2.49                     | 0.47              |
| 25:RA:1872:A:H5'   | 25:RA:1878:G:OP2   | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:231:HIS:ND1  | 27:RD:232:PRO:HD2  | 2.30                     | 0.47              |
| 29:RF:31:HIS:O     | 29:RF:34:TRP:HB3   | 2.15                     | 0.47              |
| 29:RF:65:TRP:CH2   | 29:RF:72:ARG:HB3   | 2.50                     | 0.47              |
| 30:RG:16:ARG:NH2   | 30:RG:28:VAL:O     | 2.48                     | 0.47              |
| 30:RG:44:GLY:HA2   | 30:RG:88:ILE:HG12  | 1.97                     | 0.47              |
| 32:RI:98:ALA:HB2   | 32:RI:111:PRO:HB3  | 1.96                     | 0.47              |
| 34:RO:104:ARG:HD3  | 39:RT:36:GLU:OE2   | 2.15                     | 0.47              |
| 38:RS:52:SER:O     | 38:RS:56:LEU:CD2   | 2.60                     | 0.47              |
| 38:RS:61:ASN:O     | 38:RS:65:VAL:HG23  | 2.15                     | 0.47              |
| 45:RZ:151:HIS:HA   | 45:RZ:170:THR:HA   | 1.95                     | 0.47              |
| 51:R5:56:LYS:O     | 51:R5:57:VAL:C     | 2.57                     | 0.47              |
| 52:R6:48:VAL:O     | 52:R6:49:HIS:HB2   | 2.15                     | 0.47              |
| 53:R7:25:PRO:HA    | 53:R7:28:ARG:CZ    | 2.45                     | 0.47              |
| 54:R8:56:GLU:C     | 54:R8:58:ILE:N     | 2.73                     | 0.47              |
| 1:XA:939:G:H5''    | 7:XG:102:ARG:CZ    | 2.45                     | 0.47              |
| 4:XD:31:CYS:O      | 4:XD:32:ALA:CB     | 2.62                     | 0.47              |
| 6:XF:69:GLU:O      | 6:XF:71:ARG:N      | 2.48                     | 0.47              |
| 8:XH:68:ARG:HH11   | 8:XH:68:ARG:HG2    | 1.80                     | 0.47              |
| 13:XM:36:LYS:C     | 13:XM:36:LYS:CD    | 2.86                     | 0.47              |
| 16:XP:55:ARG:O     | 16:XP:56:ALA:C     | 2.57                     | 0.47              |
| 18:XR:64:ARG:O     | 18:XR:65:ILE:C     | 2.58                     | 0.47              |
| 25:YA:389:G:C6     | 35:YP:70:GLN:HB3   | 2.50                     | 0.47              |
| 25:YA:675:A:OP1    | 29:YF:63:LYS:NZ    | 2.45                     | 0.47              |
| 25:YA:1496:A:H8    | 25:YA:1577:C:O2'   | 1.98                     | 0.47              |
| 25:YA:1593:G:H2'   | 25:YA:1594:G:C8    | 2.50                     | 0.47              |
| 25:YA:2820:A:O2'   | 25:YA:2821:A:OP1   | 2.33                     | 0.47              |
| 27:YD:136:ILE:HD12 | 27:YD:136:ILE:N    | 2.30                     | 0.47              |
| 27:YD:145:VAL:O    | 27:YD:153:ALA:HA   | 2.14                     | 0.47              |
| 28:YE:61:ARG:O     | 28:YE:63:LEU:CG    | 2.57                     | 0.47              |
| 28:YE:101:ARG:HD2  | 28:YE:171:GLU:HA   | 1.97                     | 0.47              |
| 28:YE:120:TRP:O    | 28:YE:121:ASN:HB2  | 2.15                     | 0.47              |
| 28:YE:188:VAL:O    | 28:YE:188:VAL:HG13 | 2.15                     | 0.47              |
| 30:YG:36:LYS:HA    | 30:YG:95:ARG:HG2   | 1.96                     | 0.47              |
| 30:YG:52:ILE:HG22  | 30:YG:52:ILE:O     | 2.15                     | 0.47              |
| 30:YG:104:GLU:OE1  | 50:Y4:23:GLU:HB3   | 2.15                     | 0.47              |
| 31:YH:89:ILE:HD13  | 31:YH:89:ILE:H     | 1.80                     | 0.47              |
| 36:YQ:87:LYS:O     | 36:YQ:89:ASN:N     | 2.43                     | 0.47              |
| 37:YR:28:LEU:HD13  | 37:YR:28:LEU:C     | 2.40                     | 0.47              |
| 38:YS:19:LYS:O     | 38:YS:20:ARG:CB    | 2.55                     | 0.47              |
| 40:YU:27:LEU:O     | 40:YU:30:LYS:N     | 2.41                     | 0.47              |
| 50:Y4:15:ILE:HG22  | 50:Y4:20:ASN:CA    | 2.45                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:QA:545:C:OP2   | 4:QD:62:GLN:NE2    | 2.47                     | 0.46              |
| 1:QA:1239:A:O2'  | 1:QA:1298:C:N4     | 2.48                     | 0.46              |
| 2:QB:67:THR:C    | 2:QB:68:ILE:HD12   | 2.40                     | 0.46              |
| 2:QB:174:VAL:O   | 2:QB:178:ARG:HB3   | 2.16                     | 0.46              |
| 4:QD:30:LYS:CD   | 4:QD:30:LYS:N      | 2.73                     | 0.46              |
| 5:QE:63:ARG:C    | 5:QE:66:MET:HE2    | 2.39                     | 0.46              |
| 7:QG:95:ARG:O    | 7:QG:96:GLN:C      | 2.58                     | 0.46              |
| 8:QH:28:ALA:CB   | 8:QH:57:PRO:HB2    | 2.45                     | 0.46              |
| 8:QH:74:PRO:O    | 8:QH:75:ARG:C      | 2.58                     | 0.46              |
| 10:QJ:80:LYS:NZ  | 10:QJ:80:LYS:HB2   | 2.30                     | 0.46              |
| 17:QQ:29:HIS:N   | 17:QQ:33:GLY:O     | 2.47                     | 0.46              |
| 18:QR:46:GLU:HG3 | 18:QR:47:THR:N     | 2.29                     | 0.46              |
| 20:QT:49:ALA:HB2 | 20:QT:99:LEU:HD22  | 1.97                     | 0.46              |
| 25:RA:262:A:H2'  | 25:RA:263:C:O4'    | 2.15                     | 0.46              |
| 25:RA:747:U:C4   | 25:RA:2613:U:C4    | 3.02                     | 0.46              |
| 25:RA:862:G:H2'  | 25:RA:863:A:O4'    | 2.15                     | 0.46              |
| 25:RA:871:U:H4'  | 36:RQ:69:PHE:CE2   | 2.50                     | 0.46              |
| 25:RA:1028:A:N6  | 25:RA:1125:G:H2'   | 2.30                     | 0.46              |
| 25:RA:1181:C:H2' | 25:RA:1182:A:C8    | 2.50                     | 0.46              |
| 25:RA:2612:C:C4  | 25:RA:2613:U:H5    | 2.32                     | 0.46              |
| 27:RD:18:VAL:CG1 | 27:RD:19:ALA:N     | 2.78                     | 0.46              |
| 28:RE:87:GLU:O   | 28:RE:89:ASP:N     | 2.48                     | 0.46              |
| 30:RG:98:ARG:CA  | 30:RG:101:ILE:HG12 | 2.40                     | 0.46              |
| 31:RH:18:GLU:HA  | 31:RH:18:GLU:OE2   | 2.15                     | 0.46              |
| 31:RH:41:MET:HG3 | 31:RH:54:ARG:HA    | 1.96                     | 0.46              |
| 32:RI:41:GLU:HA  | 32:RI:44:LEU:HB2   | 1.97                     | 0.46              |
| 33:RN:9:VAL:HG21 | 33:RN:48:MET:CB    | 2.45                     | 0.46              |
| 38:RS:99:LYS:C   | 38:RS:101:LEU:N    | 2.72                     | 0.46              |
| 44:RY:68:HIS:O   | 44:RY:71:LYS:HB2   | 2.15                     | 0.46              |
| 50:R4:53:GLU:O   | 50:R4:57:GLU:HG3   | 2.14                     | 0.46              |
| 53:R7:2:LYS:HG2  | 53:R7:3:ARG:N      | 2.31                     | 0.46              |
| 1:XA:1020:U:H2'  | 1:XA:1021:G:C8     | 2.49                     | 0.46              |
| 1:XA:1074:G:H4'  | 2:XB:104:ASN:HB2   | 1.96                     | 0.46              |
| 3:XC:113:ALA:C   | 3:XC:115:LEU:N     | 2.72                     | 0.46              |
| 4:XD:146:ILE:N   | 4:XD:146:ILE:CD1   | 2.73                     | 0.46              |
| 7:XG:140:ASP:HA  | 7:XG:143:ARG:HH11  | 1.79                     | 0.46              |
| 12:XL:120:TYR:O  | 12:XL:121:GLY:C    | 2.57                     | 0.46              |
| 12:XL:127:GLU:O  | 12:XL:128:ALA:CB   | 2.62                     | 0.46              |
| 18:XR:53:ARG:C   | 18:XR:55:ARG:H     | 2.22                     | 0.46              |
| 20:XT:99:LEU:O   | 20:XT:100:ILE:HB   | 2.14                     | 0.46              |
| 25:YA:1103:A:H5' | 25:YA:1104:C:C5    | 2.44                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1917:U:O4    | 25:YA:1918:A:N6    | 2.48                     | 0.46              |
| 25:YA:2405:G:HO2'  | 25:YA:2406:U:P     | 2.35                     | 0.46              |
| 30:YG:13:GLU:O     | 30:YG:13:GLU:HG3   | 2.14                     | 0.46              |
| 30:YG:135:LEU:HD11 | 30:YG:157:ILE:HD12 | 1.98                     | 0.46              |
| 32:YI:33:ARG:O     | 32:YI:35:LEU:HG    | 2.14                     | 0.46              |
| 33:YN:35:ARG:HG3   | 33:YN:35:ARG:O     | 2.15                     | 0.46              |
| 34:YO:50:GLY:O     | 34:YO:51:ALA:C     | 2.57                     | 0.46              |
| 35:YP:46:LYS:O     | 35:YP:48:PRO:N     | 2.48                     | 0.46              |
| 36:YQ:34:LEU:HD11  | 36:YQ:129:THR:CB   | 2.35                     | 0.46              |
| 37:YR:1:MET:O      | 37:YR:2:ARG:HB2    | 2.15                     | 0.46              |
| 38:YS:24:LEU:HB2   | 38:YS:85:VAL:HG12  | 1.97                     | 0.46              |
| 40:YU:27:LEU:C     | 40:YU:29:SER:N     | 2.74                     | 0.46              |
| 43:YX:14:SER:O     | 43:YX:15:GLU:C     | 2.57                     | 0.46              |
| 43:YX:26:TYR:HB3   | 43:YX:92:LEU:HD12  | 1.97                     | 0.46              |
| 44:YY:81:LYS:NZ    | 44:YY:98:VAL:HB    | 2.30                     | 0.46              |
| 47:Y1:81:LYS:HE2   | 47:Y1:81:LYS:H     | 1.62                     | 0.46              |
| 51:Y5:45:VAL:HG12  | 51:Y5:45:VAL:O     | 2.13                     | 0.46              |
| 54:Y8:9:GLY:O      | 54:Y8:13:ARG:HG2   | 2.15                     | 0.46              |
| 54:Y8:40:GLU:O     | 54:Y8:41:ILE:C     | 2.56                     | 0.46              |
| 1:QA:519:C:H2'     | 1:QA:520:A:O4'     | 2.15                     | 0.46              |
| 1:QA:1151:A:N3     | 10:QJ:39:PRO:HG3   | 2.30                     | 0.46              |
| 3:QC:172:ARG:O     | 3:QC:173:VAL:HG23  | 2.15                     | 0.46              |
| 9:QI:22:GLY:O      | 9:QI:23:ASN:C      | 2.57                     | 0.46              |
| 15:QO:82:ILE:O     | 15:QO:86:GLY:N     | 2.49                     | 0.46              |
| 19:QS:40:ILE:CG1   | 19:QS:41:VAL:N     | 2.78                     | 0.46              |
| 20:QT:26:ASN:N     | 20:QT:26:ASN:ND2   | 2.62                     | 0.46              |
| 20:QT:53:LEU:HD12  | 20:QT:100:ILE:HG23 | 1.98                     | 0.46              |
| 25:RA:38:A:H2'     | 25:RA:39:C:C6      | 2.50                     | 0.46              |
| 25:RA:588:U:H1'    | 29:RF:90:PHE:CD1   | 2.50                     | 0.46              |
| 25:RA:1657:C:H2'   | 25:RA:1658:C:H6    | 1.79                     | 0.46              |
| 25:RA:2290:G:H1    | 25:RA:2342:C:H42   | 1.63                     | 0.46              |
| 25:RA:2566:A:H4'   | 25:RA:2567:G:O5'   | 2.14                     | 0.46              |
| 25:RA:2712:U:O2'   | 25:RA:2712(A):A:C8 | 2.68                     | 0.46              |
| 26:RB:48:A:H4'     | 38:RS:95:HIS:CD2   | 2.49                     | 0.46              |
| 27:RD:27:THR:O     | 27:RD:29:PRO:CD    | 2.62                     | 0.46              |
| 27:RD:110:GLY:O    | 27:RD:111:LEU:C    | 2.59                     | 0.46              |
| 27:RD:183:ARG:CG   | 27:RD:183:ARG:NH1  | 2.69                     | 0.46              |
| 29:RF:61:GLY:O     | 29:RF:62:ARG:C     | 2.58                     | 0.46              |
| 31:RH:127:GLU:OE2  | 31:RH:130:ARG:NH2  | 2.47                     | 0.46              |
| 32:RI:5:LEU:HD11   | 32:RI:19:VAL:HG12  | 1.96                     | 0.46              |
| 33:RN:27:ALA:O     | 33:RN:28:THR:C     | 2.57                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:RO:50:GLY:O     | 34:RO:51:ALA:C     | 2.57                     | 0.46              |
| 35:RP:37:GLY:O     | 35:RP:38:GLN:C     | 2.58                     | 0.46              |
| 37:RR:56:LYS:HE2   | 37:RR:94:TYR:OH    | 2.15                     | 0.46              |
| 37:RR:78:LYS:O     | 37:RR:78:LYS:HG2   | 2.15                     | 0.46              |
| 38:RS:42:ASP:C     | 38:RS:44:LYS:N     | 2.72                     | 0.46              |
| 43:RX:87:GLN:C     | 43:RX:88:LYS:HG3   | 2.40                     | 0.46              |
| 47:R1:49:VAL:HG12  | 47:R1:51:VAL:CG2   | 2.45                     | 0.46              |
| 47:R1:76:ARG:HD2   | 47:R1:76:ARG:N     | 2.29                     | 0.46              |
| 48:R2:7:ARG:HG3    | 48:R2:7:ARG:NH1    | 2.25                     | 0.46              |
| 50:R4:61:ARG:C     | 50:R4:63:TYR:N     | 2.73                     | 0.46              |
| 54:R8:29:LYS:HE3   | 54:R8:41:ILE:O     | 2.15                     | 0.46              |
| 1:XA:265:G:H2'     | 1:XA:266:G:H5''    | 1.98                     | 0.46              |
| 1:XA:811:C:H4'     | 1:XA:900:A:N6      | 2.30                     | 0.46              |
| 1:XA:1346:A:C5     | 7:XG:10:ARG:NH1    | 2.84                     | 0.46              |
| 2:XB:15:VAL:HG23   | 2:XB:209:ARG:HE    | 1.80                     | 0.46              |
| 2:XB:174:VAL:O     | 2:XB:178:ARG:HB3   | 2.15                     | 0.46              |
| 3:XC:11:ARG:HG2    | 3:XC:11:ARG:HH11   | 1.79                     | 0.46              |
| 3:XC:23:TYR:CG     | 3:XC:24:ALA:N      | 2.83                     | 0.46              |
| 4:XD:110:PHE:HD1   | 4:XD:110:PHE:H     | 1.62                     | 0.46              |
| 4:XD:135:LEU:O     | 4:XD:137:SER:N     | 2.48                     | 0.46              |
| 7:XG:95:ARG:O      | 7:XG:96:GLN:C      | 2.58                     | 0.46              |
| 18:XR:31:LEU:HD23  | 18:XR:31:LEU:N     | 2.29                     | 0.46              |
| 19:XS:40:ILE:CG1   | 19:XS:41:VAL:N     | 2.78                     | 0.46              |
| 19:XS:64:GLU:HB2   | 50:Y4:55:ARG:HH12  | 1.80                     | 0.46              |
| 25:YA:273(F):C:H2' | 25:YA:274:G:H5''   | 1.98                     | 0.46              |
| 25:YA:871:U:H4'    | 36:YQ:69:PHE:CE2   | 2.50                     | 0.46              |
| 25:YA:1022:G:C6    | 25:YA:1140:C:C4    | 3.03                     | 0.46              |
| 25:YA:1266:G:O2'   | 25:YA:2012:G:O6    | 2.28                     | 0.46              |
| 25:YA:1705:G:C6    | 25:YA:1706:U:C4    | 3.04                     | 0.46              |
| 25:YA:2059:A:H5'   | 25:YA:2060:A:OP2   | 2.16                     | 0.46              |
| 27:YD:102:LYS:O    | 27:YD:103:ARG:HG3  | 2.15                     | 0.46              |
| 31:YH:9:ILE:O      | 31:YH:10:PRO:O     | 2.33                     | 0.46              |
| 31:YH:104:GLU:HG3  | 31:YH:114:VAL:HG22 | 1.96                     | 0.46              |
| 32:YI:128:LEU:N    | 32:YI:138:ILE:O    | 2.48                     | 0.46              |
| 34:YO:104:ARG:HG2  | 34:YO:121:VAL:HG12 | 1.97                     | 0.46              |
| 35:YP:37:GLY:O     | 35:YP:41:ARG:HD3   | 2.15                     | 0.46              |
| 36:YQ:109:VAL:HG13 | 36:YQ:113:GLN:OE1  | 2.16                     | 0.46              |
| 38:YS:28:VAL:HG11  | 38:YS:98:VAL:HG12  | 1.97                     | 0.46              |
| 39:YT:111:ARG:C    | 39:YT:113:LYS:N    | 2.64                     | 0.46              |
| 41:YV:6:LYS:HD3    | 41:YV:11:GLN:HG2   | 1.96                     | 0.46              |
| 42:YW:36:LEU:CD1   | 42:YW:47:VAL:HG12  | 2.44                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:YY:68:HIS:O    | 44:YY:71:LYS:HB2  | 2.15                     | 0.46              |
| 47:Y1:76:ARG:H    | 47:Y1:76:ARG:CD   | 2.29                     | 0.46              |
| 1:QA:218:C:H2'    | 1:QA:219:C:C6     | 2.50                     | 0.46              |
| 1:QA:778:G:H2'    | 1:QA:779:C:O4'    | 2.15                     | 0.46              |
| 1:QA:1053:G:H2'   | 1:QA:1199:U:C5    | 2.49                     | 0.46              |
| 1:QA:1512:U:H2'   | 1:QA:1513:A:C8    | 2.50                     | 0.46              |
| 2:QB:17:PHE:CD2   | 2:QB:44:LEU:HD21  | 2.47                     | 0.46              |
| 7:QG:92:SER:HB3   | 7:QG:95:ARG:CB    | 2.45                     | 0.46              |
| 10:QJ:47:PHE:CE1  | 10:QJ:63:PHE:HB2  | 2.32                     | 0.46              |
| 10:QJ:49:VAL:HG22 | 14:QN:41:ARG:CD   | 2.45                     | 0.46              |
| 10:QJ:95:GLU:OE2  | 10:QJ:95:GLU:HA   | 2.16                     | 0.46              |
| 13:QM:65:LYS:NZ   | 13:QM:69:GLU:HG2  | 2.30                     | 0.46              |
| 13:QM:80:ARG:O    | 13:QM:82:MET:O    | 2.34                     | 0.46              |
| 19:QS:24:ALA:O    | 19:QS:25:LYS:CB   | 2.63                     | 0.46              |
| 22:QV:35:A:C2     | 24:QX:3:G:C2      | 3.04                     | 0.46              |
| 25:RA:99:U:H4'    | 25:RA:101:G:O5'   | 2.16                     | 0.46              |
| 25:RA:583:G:H5''  | 40:RU:10:ARG:NH1  | 2.28                     | 0.46              |
| 25:RA:612:G:H2'   | 25:RA:613:U:O2    | 2.16                     | 0.46              |
| 25:RA:858:U:O2    | 25:RA:2268:A:H2'  | 2.15                     | 0.46              |
| 25:RA:2696:U:H2'  | 25:RA:2697:G:C8   | 2.50                     | 0.46              |
| 26:RB:42:C:O4'    | 30:RG:69:ALA:HB2  | 2.15                     | 0.46              |
| 27:RD:35:LYS:HD3  | 27:RD:63:ARG:HB3  | 1.96                     | 0.46              |
| 30:RG:60:LEU:HD23 | 30:RG:60:LEU:C    | 2.41                     | 0.46              |
| 31:RH:9:ILE:O     | 31:RH:10:PRO:O    | 2.33                     | 0.46              |
| 31:RH:153:LYS:HG3 | 31:RH:162:ILE:H   | 1.78                     | 0.46              |
| 34:RO:112:MET:O   | 34:RO:115:VAL:CG2 | 2.64                     | 0.46              |
| 38:RS:26:LEU:HD22 | 38:RS:87:PHE:CD1  | 2.46                     | 0.46              |
| 38:RS:28:VAL:HG11 | 38:RS:98:VAL:HG12 | 1.97                     | 0.46              |
| 39:RT:29:ARG:NH1  | 39:RT:46:GLU:OE1  | 2.48                     | 0.46              |
| 41:RV:30:GLY:O    | 41:RV:31:ALA:O    | 2.34                     | 0.46              |
| 43:RX:12:VAL:O    | 43:RX:12:VAL:HG13 | 2.15                     | 0.46              |
| 44:RY:15:VAL:O    | 44:RY:21:LYS:HA   | 2.15                     | 0.46              |
| 49:R3:56:VAL:CG1  | 49:R3:57:GLU:N    | 2.74                     | 0.46              |
| 51:R5:43:HIS:N    | 51:R5:43:HIS:ND1  | 2.63                     | 0.46              |
| 2:XB:77:ALA:HB1   | 2:XB:211:ILE:HG21 | 1.97                     | 0.46              |
| 3:XC:73:PRO:O     | 3:XC:77:ILE:HG13  | 2.16                     | 0.46              |
| 3:XC:134:ILE:HG23 | 3:XC:151:VAL:HB   | 1.98                     | 0.46              |
| 3:XC:172:ARG:O    | 3:XC:173:VAL:CG2  | 2.63                     | 0.46              |
| 8:XH:80:ILE:HG23  | 8:XH:137:VAL:HG12 | 1.97                     | 0.46              |
| 9:XI:17:VAL:HG11  | 9:XI:81:ILE:HA    | 1.96                     | 0.46              |
| 13:XM:68:GLY:CA   | 30:YG:116:ASP:OD2 | 2.63                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:XU:2:GLY:C     | 21:XU:4:GLY:H      | 2.23                     | 0.46              |
| 25:YA:1228:G:OP1  | 40:YU:13:LYS:HG2   | 2.16                     | 0.46              |
| 25:YA:1826:G:O2'  | 27:YD:242:ARG:NH2  | 2.48                     | 0.46              |
| 25:YA:1869:G:H5'  | 25:YA:1870:C:OP2   | 2.14                     | 0.46              |
| 25:YA:2322:A:H2'  | 25:YA:2323:G:O4'   | 2.16                     | 0.46              |
| 27:YD:110:GLY:O   | 27:YD:111:LEU:C    | 2.58                     | 0.46              |
| 28:YE:7:VAL:HG11  | 39:YT:1:MET:CE     | 2.45                     | 0.46              |
| 30:YG:116:ASP:O   | 30:YG:117:PHE:CB   | 2.50                     | 0.46              |
| 31:YH:86:GLU:O    | 31:YH:132:ARG:HA   | 2.16                     | 0.46              |
| 31:YH:94:TYR:N    | 31:YH:94:TYR:CD1   | 2.82                     | 0.46              |
| 32:YI:100:ALA:O   | 32:YI:104:GLN:HB2  | 2.15                     | 0.46              |
| 34:YO:7:TYR:CD1   | 34:YO:20:MET:HB2   | 2.50                     | 0.46              |
| 34:YO:61:VAL:O    | 34:YO:84:ALA:HB1   | 2.16                     | 0.46              |
| 37:YR:10:LEU:C    | 37:YR:12:ARG:N     | 2.72                     | 0.46              |
| 37:YR:79:LEU:HD23 | 37:YR:79:LEU:O     | 2.16                     | 0.46              |
| 39:YT:118:ARG:NH2 | 39:YT:121:ILE:HD12 | 2.31                     | 0.46              |
| 40:YU:57:PHE:C    | 40:YU:59:ARG:N     | 2.74                     | 0.46              |
| 41:YV:5:VAL:HG13  | 41:YV:14:VAL:HG21  | 1.98                     | 0.46              |
| 42:YW:17:VAL:O    | 42:YW:18:ARG:C     | 2.57                     | 0.46              |
| 43:YX:12:VAL:O    | 43:YX:12:VAL:HG13  | 2.15                     | 0.46              |
| 54:Y8:29:LYS:HE3  | 54:Y8:41:ILE:O     | 2.15                     | 0.46              |
| 1:QA:1053:G:H2'   | 1:QA:1199:U:H5     | 1.80                     | 0.46              |
| 3:QC:108:ASN:HB3  | 3:QC:111:LEU:HG    | 1.98                     | 0.46              |
| 5:QE:12:LEU:HD21  | 5:QE:14:ARG:HB3    | 1.98                     | 0.46              |
| 5:QE:55:VAL:O     | 5:QE:58:ALA:HB3    | 2.16                     | 0.46              |
| 5:QE:153:LYS:HD3  | 5:QE:153:LYS:C     | 2.41                     | 0.46              |
| 6:QF:3:ARG:HG3    | 6:QF:3:ARG:HH11    | 1.80                     | 0.46              |
| 7:QG:50:ILE:CG2   | 7:QG:61:VAL:HG21   | 2.45                     | 0.46              |
| 12:QL:43:VAL:HG23 | 12:QL:93:LEU:HD22  | 1.96                     | 0.46              |
| 13:QM:23:TYR:HB2  | 13:QM:67:GLU:OE1   | 2.15                     | 0.46              |
| 16:QP:25:ARG:HG3  | 16:QP:25:ARG:HH11  | 1.79                     | 0.46              |
| 20:QT:99:LEU:O    | 20:QT:100:ILE:HB   | 2.15                     | 0.46              |
| 25:RA:265:A:O2'   | 25:RA:266:G:H4'    | 2.16                     | 0.46              |
| 25:RA:299:A:C5'   | 44:RY:84:ARG:HH21  | 2.28                     | 0.46              |
| 26:RB:11:C:H3'    | 26:RB:12:C:H6      | 1.80                     | 0.46              |
| 27:RD:27:THR:CG2  | 27:RD:28:GLU:N     | 2.66                     | 0.46              |
| 28:RE:54:GLN:CA   | 28:RE:54:GLN:HE21  | 2.27                     | 0.46              |
| 28:RE:94:GLU:C    | 28:RE:96:PHE:N     | 2.73                     | 0.46              |
| 31:RH:4:ILE:H     | 31:RH:4:ILE:CD1    | 2.25                     | 0.46              |
| 35:RP:81:GLN:HB3  | 35:RP:110:TYR:HB3  | 1.97                     | 0.46              |
| 38:RS:13:ARG:O    | 38:RS:14:VAL:HB    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:RV:81:TYR:C    | 41:RV:82:ARG:CG    | 2.89                     | 0.46              |
| 42:RW:4:LYS:HA    | 42:RW:106:ILE:HA   | 1.97                     | 0.46              |
| 43:RX:24:GLY:O    | 43:RX:82:GLN:HA    | 2.16                     | 0.46              |
| 44:RY:35:TYR:CD1  | 44:RY:35:TYR:O     | 2.69                     | 0.46              |
| 45:RZ:74:VAL:HG13 | 45:RZ:86:VAL:HG22  | 1.97                     | 0.46              |
| 47:R1:79:GLY:N    | 47:R1:80:LEU:HD23  | 2.30                     | 0.46              |
| 1:XA:109:A:C6     | 1:XA:326:G:C6      | 3.03                     | 0.46              |
| 1:XA:474:G:H5'    | 16:XP:81:ARG:HG3   | 1.96                     | 0.46              |
| 1:XA:677:U:H1'    | 11:XK:119:CYS:SG   | 2.55                     | 0.46              |
| 3:XC:113:ALA:O    | 3:XC:115:LEU:N     | 2.48                     | 0.46              |
| 8:XH:122:ARG:O    | 8:XH:125:ARG:N     | 2.46                     | 0.46              |
| 9:XI:9:ARG:HA     | 9:XI:76:ALA:HB1    | 1.96                     | 0.46              |
| 10:XJ:38:ILE:CD1  | 10:XJ:71:LEU:HB3   | 2.46                     | 0.46              |
| 11:XK:80:VAL:O    | 11:XK:106:LYS:HD3  | 2.16                     | 0.46              |
| 15:XO:50:HIS:O    | 15:XO:53:HIS:N     | 2.47                     | 0.46              |
| 15:XO:77:ARG:HA   | 15:XO:80:ALA:HB3   | 1.96                     | 0.46              |
| 16:XP:60:LEU:CA   | 16:XP:64:ALA:HB3   | 2.43                     | 0.46              |
| 17:XQ:100:LYS:O   | 17:XQ:101:ARG:HB2  | 2.15                     | 0.46              |
| 21:XU:14:TRP:CE3  | 21:XU:15:ARG:NH1   | 2.83                     | 0.46              |
| 25:YA:851:U:O2'   | 49:Y3:45:GLY:HA3   | 2.16                     | 0.46              |
| 25:YA:1028:A:H2'  | 25:YA:1029:A:C8    | 2.51                     | 0.46              |
| 27:YD:211:ARG:HG2 | 27:YD:211:ARG:HH11 | 1.80                     | 0.46              |
| 29:YF:46:ARG:CG   | 29:YF:46:ARG:NH1   | 2.71                     | 0.46              |
| 29:YF:183:VAL:O   | 29:YF:184:TYR:C    | 2.57                     | 0.46              |
| 30:YG:102:PHE:HA  | 30:YG:105:LYS:HE3  | 1.98                     | 0.46              |
| 31:YH:4:ILE:HG13  | 31:YH:6:ARG:HD3    | 1.97                     | 0.46              |
| 32:YI:90:GLY:O    | 32:YI:121:LYS:HE2  | 2.15                     | 0.46              |
| 33:YN:30:ILE:O    | 33:YN:34:LEU:CD2   | 2.63                     | 0.46              |
| 33:YN:46:VAL:HG13 | 33:YN:47:ALA:N     | 2.31                     | 0.46              |
| 33:YN:96:GLU:O    | 33:YN:99:LEU:N     | 2.34                     | 0.46              |
| 35:YP:144:GLU:OE1 | 35:YP:144:GLU:N    | 2.48                     | 0.46              |
| 35:YP:144:GLU:HA  | 35:YP:145:PRO:HD3  | 1.76                     | 0.46              |
| 37:YR:78:LYS:HG2  | 37:YR:78:LYS:O     | 2.15                     | 0.46              |
| 37:YR:85:PRO:C    | 37:YR:87:TYR:N     | 2.73                     | 0.46              |
| 39:YT:96:ARG:CB   | 39:YT:96:ARG:HH11  | 2.29                     | 0.46              |
| 48:Y2:4:SER:OG    | 48:Y2:5:GLU:OE2    | 2.26                     | 0.46              |
| 55:Y9:19:ARG:NH2  | 55:Y9:26:ILE:HD11  | 2.31                     | 0.46              |
| 1:QA:1271:G:H5'   | 1:QA:1314:C:H5'    | 1.96                     | 0.46              |
| 1:QA:1321:C:C4    | 1:QA:1322:C:C4     | 3.04                     | 0.46              |
| 1:QA:1329:A:H5''  | 13:QM:29:ARG:HG3   | 1.96                     | 0.46              |
| 1:QA:1521:G:H2'   | 1:QA:1522:U:C6     | 2.50                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:QB:155:LEU:C    | 2:QB:157:ARG:H     | 2.23                     | 0.46              |
| 2:QB:224:GLN:HA   | 2:QB:229:VAL:HG23  | 1.97                     | 0.46              |
| 3:QC:95:THR:CG2   | 3:QC:97:LYS:HZ3    | 2.29                     | 0.46              |
| 5:QE:13:ILE:HG22  | 5:QE:13:ILE:O      | 2.14                     | 0.46              |
| 6:QF:68:PRO:HG3   | 6:QF:71:ARG:NH2    | 2.31                     | 0.46              |
| 9:QI:59:PHE:CZ    | 9:QI:88:TYR:CE1    | 3.01                     | 0.46              |
| 10:QJ:44:VAL:HG12 | 10:QJ:45:ARG:N     | 2.30                     | 0.46              |
| 10:QJ:63:PHE:CD1  | 14:QN:58:LYS:HA    | 2.35                     | 0.46              |
| 11:QK:70:LYS:HA   | 11:QK:73:MET:HE3   | 1.98                     | 0.46              |
| 12:QL:115:LYS:O   | 12:QL:117:ARG:N    | 2.47                     | 0.46              |
| 14:QN:41:ARG:HH11 | 14:QN:41:ARG:HG2   | 1.79                     | 0.46              |
| 18:QR:20:ALA:C    | 18:QR:21:LYS:HG3   | 2.41                     | 0.46              |
| 25:RA:476:G:N1    | 25:RA:479:A:OP2    | 2.46                     | 0.46              |
| 25:RA:896:A:C2    | 45:RZ:146:ILE:HD11 | 2.50                     | 0.46              |
| 25:RA:2283:C:H2'  | 25:RA:2284:C:O4'   | 2.15                     | 0.46              |
| 25:RA:2331:G:H4'  | 46:R0:43:THR:N     | 2.31                     | 0.46              |
| 27:RD:61:LEU:HB3  | 27:RD:63:ARG:NH1   | 2.31                     | 0.46              |
| 28:RE:188:VAL:O   | 28:RE:188:VAL:HG13 | 2.15                     | 0.46              |
| 31:RH:86:GLU:O    | 31:RH:132:ARG:HA   | 2.15                     | 0.46              |
| 35:RP:125:VAL:C   | 35:RP:145:PRO:HD2  | 2.39                     | 0.46              |
| 37:RR:29:LEU:N    | 37:RR:29:LEU:CD1   | 2.79                     | 0.46              |
| 37:RR:75:LEU:HA   | 37:RR:78:LYS:HB3   | 1.97                     | 0.46              |
| 38:RS:66:ALA:HA   | 38:RS:69:VAL:HG12  | 1.96                     | 0.46              |
| 47:R1:83:GLU:OE1  | 47:R1:85:LEU:HB2   | 2.15                     | 0.46              |
| 49:R3:18:ASP:O    | 49:R3:21:ALA:N     | 2.49                     | 0.46              |
| 50:R4:64:GLY:C    | 50:R4:66:SER:N     | 2.73                     | 0.46              |
| 52:R6:18:ARG:O    | 52:R6:19:ARG:O     | 2.33                     | 0.46              |
| 54:R8:52:LYS:O    | 54:R8:52:LYS:CG    | 2.64                     | 0.46              |
| 1:XA:502:G:C6     | 1:XA:503:C:C4      | 3.03                     | 0.46              |
| 1:XA:673:G:H2'    | 1:XA:674:G:C8      | 2.50                     | 0.46              |
| 1:XA:1119:C:H2'   | 1:XA:1120:G:C8     | 2.50                     | 0.46              |
| 3:XC:108:ASN:CG   | 3:XC:111:LEU:HG    | 2.41                     | 0.46              |
| 6:XF:41:GLU:HG2   | 6:XF:43:LEU:CD1    | 2.44                     | 0.46              |
| 8:XH:49:GLU:HG3   | 8:XH:49:GLU:O      | 2.14                     | 0.46              |
| 8:XH:86:ILE:CG1   | 8:XH:133:LEU:HD22  | 2.46                     | 0.46              |
| 10:XJ:80:LYS:HB2  | 10:XJ:80:LYS:NZ    | 2.31                     | 0.46              |
| 11:XK:34:ASP:HB2  | 11:XK:35:PRO:CD    | 2.45                     | 0.46              |
| 13:XM:23:TYR:HB3  | 13:XM:67:GLU:HA    | 1.98                     | 0.46              |
| 17:XQ:92:ARG:HG3  | 17:XQ:92:ARG:NH1   | 2.30                     | 0.46              |
| 20:XT:48:LYS:O    | 20:XT:49:ALA:C     | 2.59                     | 0.46              |
| 20:XT:96:GLY:O    | 20:XT:99:LEU:HD13  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:105:C:H2'    | 25:YA:106:C:H6    | 1.80                     | 0.46              |
| 25:YA:1398:C:OP1   | 43:YX:53:LYS:NZ   | 2.49                     | 0.46              |
| 25:YA:1407:C:H5'   | 25:YA:1408:C:OP2  | 2.16                     | 0.46              |
| 25:YA:1932:A:H2'   | 25:YA:1933:G:O4'  | 2.16                     | 0.46              |
| 25:YA:2046:G:H2'   | 25:YA:2047:U:H6   | 1.80                     | 0.46              |
| 25:YA:2573:C:N4    | 56:Z8:75:C:HO2'   | 2.14                     | 0.46              |
| 26:YB:66:A:O2'     | 26:YB:67:G:O5'    | 2.33                     | 0.46              |
| 27:YD:183:ARG:CG   | 27:YD:183:ARG:NH1 | 2.69                     | 0.46              |
| 27:YD:206:LEU:HD23 | 27:YD:206:LEU:HA  | 1.49                     | 0.46              |
| 30:YG:20:ILE:HD13  | 30:YG:25:TYR:HB2  | 1.98                     | 0.46              |
| 33:YN:114:ARG:C    | 33:YN:116:LEU:N   | 2.74                     | 0.46              |
| 33:YN:131:GLN:HE21 | 33:YN:132:ALA:H   | 1.58                     | 0.46              |
| 34:YO:92:GLU:O     | 34:YO:93:PRO:C    | 2.58                     | 0.46              |
| 35:YP:1:MET:O      | 35:YP:2:LYS:HG3   | 2.16                     | 0.46              |
| 36:YQ:63:LYS:HE2   | 36:YQ:65:PHE:CZ   | 2.50                     | 0.46              |
| 36:YQ:66:ILE:H     | 36:YQ:104:PHE:HA  | 1.79                     | 0.46              |
| 40:YU:73:GLY:O     | 40:YU:74:LEU:CB   | 2.63                     | 0.46              |
| 41:YV:81:TYR:C     | 41:YV:82:ARG:CG   | 2.89                     | 0.46              |
| 43:YX:65:ARG:N     | 43:YX:65:ARG:CD   | 2.79                     | 0.46              |
| 49:Y3:28:LEU:HA    | 49:Y3:33:GLN:OE1  | 2.16                     | 0.46              |
| 49:Y3:39:ASP:O     | 49:Y3:40:THR:C    | 2.59                     | 0.46              |
| 49:Y3:59:VAL:CG1   | 49:Y3:60:GLU:H    | 2.28                     | 0.46              |
| 51:Y5:39:MET:C     | 51:Y5:40:LYS:HG3  | 2.39                     | 0.46              |
| 52:Y6:15:GLU:HB3   | 52:Y6:16:CYS:H    | 1.46                     | 0.46              |
| 1:QA:164:U:H2'     | 1:QA:165:C:H6     | 1.81                     | 0.46              |
| 1:QA:999:U:O2'     | 25:YA:2137:C:OP1  | 2.20                     | 0.46              |
| 1:QA:1158:C:H2'    | 1:QA:1158:C:O2    | 2.14                     | 0.46              |
| 2:QB:162:ILE:CD1   | 2:QB:184:VAL:HG13 | 2.44                     | 0.46              |
| 3:QC:15:THR:HG22   | 3:QC:15:THR:O     | 2.15                     | 0.46              |
| 3:QC:113:ALA:O     | 3:QC:115:LEU:N    | 2.48                     | 0.46              |
| 5:QE:150:ARG:HG2   | 5:QE:150:ARG:O    | 2.16                     | 0.46              |
| 7:QG:95:ARG:NE     | 7:QG:99:LEU:HD11  | 2.31                     | 0.46              |
| 8:QH:86:ILE:HG13   | 8:QH:133:LEU:CD2  | 2.44                     | 0.46              |
| 11:QK:34:ASP:HB2   | 11:QK:35:PRO:CD   | 2.45                     | 0.46              |
| 25:RA:642:G:H21    | 25:RA:646:A:H2    | 1.62                     | 0.46              |
| 25:RA:1169:G:H1    | 25:RA:1180:C:N4   | 2.12                     | 0.46              |
| 25:RA:1543:A:O2'   | 25:RA:1544:C:O5'  | 2.30                     | 0.46              |
| 25:RA:2074:U:H2'   | 25:RA:2075:U:C6   | 2.51                     | 0.46              |
| 25:RA:2292:C:P     | 38:RS:17:ARG:HH22 | 2.39                     | 0.46              |
| 28:RE:33:VAL:HG12  | 28:RE:90:THR:H    | 1.81                     | 0.46              |
| 28:RE:89:ASP:O     | 28:RE:90:THR:O    | 2.33                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:103:ASP:OD2  | 28:RE:168:MET:HG2  | 2.15                     | 0.46              |
| 35:RP:6:LEU:N      | 35:RP:6:LEU:HD22   | 2.31                     | 0.46              |
| 35:RP:45:LEU:CD1   | 35:RP:45:LEU:N     | 2.79                     | 0.46              |
| 35:RP:90:ARG:HB3   | 35:RP:91:PHE:H     | 1.60                     | 0.46              |
| 35:RP:107:LYS:O    | 35:RP:108:LYS:C    | 2.57                     | 0.46              |
| 36:RQ:66:ILE:O     | 36:RQ:104:PHE:N    | 2.49                     | 0.46              |
| 36:RQ:109:VAL:HG13 | 36:RQ:113:GLN:OE1  | 2.16                     | 0.46              |
| 39:RT:51:ARG:CG    | 39:RT:98:LYS:HG3   | 2.44                     | 0.46              |
| 39:RT:96:ARG:CB    | 39:RT:96:ARG:HH11  | 2.29                     | 0.46              |
| 39:RT:118:ARG:NH2  | 39:RT:121:ILE:HD12 | 2.31                     | 0.46              |
| 41:RV:47:VAL:O     | 41:RV:48:GLY:O     | 2.34                     | 0.46              |
| 42:RW:17:VAL:O     | 42:RW:18:ARG:C     | 2.57                     | 0.46              |
| 43:RX:8:ILE:CD1    | 43:RX:42:ALA:HB1   | 2.46                     | 0.46              |
| 49:R3:59:VAL:CG1   | 49:R3:60:GLU:H     | 2.28                     | 0.46              |
| 50:R4:15:ILE:HG22  | 50:R4:20:ASN:CA    | 2.45                     | 0.46              |
| 50:R4:50:VAL:O     | 50:R4:50:VAL:HG13  | 2.15                     | 0.46              |
| 1:XA:1016:A:H2'    | 1:XA:1017:G:O4'    | 2.15                     | 0.46              |
| 1:XA:1224:G:C6     | 1:XA:1322:C:H1'    | 2.50                     | 0.46              |
| 1:XA:1316:G:H22    | 1:XA:1319:A:H5''   | 1.81                     | 0.46              |
| 2:XB:17:PHE:CD2    | 2:XB:44:LEU:HD21   | 2.47                     | 0.46              |
| 6:XF:98:LEU:HD12   | 6:XF:98:LEU:C      | 2.41                     | 0.46              |
| 9:XI:20:ARG:O      | 9:XI:21:PRO:C      | 2.59                     | 0.46              |
| 12:XL:126:LYS:HB2  | 12:XL:126:LYS:HZ3  | 1.80                     | 0.46              |
| 16:XP:75:ARG:C     | 16:XP:77:ALA:N     | 2.72                     | 0.46              |
| 17:XQ:76:LEU:HD11  | 17:XQ:79:SER:H     | 1.80                     | 0.46              |
| 25:YA:602:G:O2'    | 25:YA:604:G:O2'    | 2.10                     | 0.46              |
| 25:YA:2009:G:OP1   | 42:YW:41:LYS:HE2   | 2.16                     | 0.46              |
| 25:YA:2062:A:H2'   | 25:YA:2062:A:N3    | 2.30                     | 0.46              |
| 25:YA:2212:A:H1'   | 25:YA:2215:G:C4    | 2.51                     | 0.46              |
| 27:YD:61:LEU:HB3   | 27:YD:63:ARG:NH1   | 2.31                     | 0.46              |
| 28:YE:3:GLY:HA3    | 28:YE:81:ILE:HG21  | 1.97                     | 0.46              |
| 28:YE:63:LEU:O     | 28:YE:64:LYS:CB    | 2.62                     | 0.46              |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:N    | 2.29                     | 0.46              |
| 29:YF:184:TYR:CD2  | 29:YF:188:ARG:HD2  | 2.50                     | 0.46              |
| 30:YG:36:LYS:O     | 30:YG:37:VAL:HG23  | 2.15                     | 0.46              |
| 30:YG:60:LEU:HD23  | 30:YG:60:LEU:C     | 2.41                     | 0.46              |
| 31:YH:86:GLU:O     | 31:YH:87:LEU:CB    | 2.64                     | 0.46              |
| 31:YH:151:ILE:O    | 31:YH:152:ARG:O    | 2.34                     | 0.46              |
| 32:YI:8:PRO:HD3    | 32:YI:15:VAL:HG13  | 1.97                     | 0.46              |
| 33:YN:27:ALA:O     | 33:YN:28:THR:C     | 2.57                     | 0.46              |
| 33:YN:28:THR:O     | 33:YN:29:LYS:C     | 2.59                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:36:GLY:O     | 33:YN:42:TRP:HE3   | 1.98                     | 0.46              |
| 34:YO:101:PRO:HA   | 34:YO:120:GLU:O    | 2.16                     | 0.46              |
| 36:YQ:80:GLU:OE1   | 46:Y0:7:LEU:HG     | 2.16                     | 0.46              |
| 39:YT:6:LEU:O      | 39:YT:10:VAL:HG23  | 2.16                     | 0.46              |
| 40:YU:69:CYS:O     | 40:YU:74:LEU:HD12  | 2.16                     | 0.46              |
| 41:YV:16:PRO:HA    | 41:YV:96:ILE:O     | 2.14                     | 0.46              |
| 41:YV:61:VAL:HA    | 41:YV:94:LEU:HD23  | 1.97                     | 0.46              |
| 47:Y1:80:LEU:CB    | 47:Y1:81:LYS:HE2   | 2.43                     | 0.46              |
| 1:QA:60:A:N6       | 1:QA:110:C:N3      | 2.60                     | 0.46              |
| 1:QA:337:C:H2'     | 1:QA:338:A:C8      | 2.51                     | 0.46              |
| 1:QA:792:A:O2'     | 1:QA:794:A:N7      | 2.40                     | 0.46              |
| 1:QA:1004:A:H1'    | 1:QA:1036:G:N2     | 2.31                     | 0.46              |
| 1:QA:1316:G:H22    | 1:QA:1319:A:C5'    | 2.29                     | 0.46              |
| 2:QB:170:GLU:CA    | 2:QB:172:ILE:HD12  | 2.46                     | 0.46              |
| 3:QC:143:GLU:C     | 3:QC:145:GLY:H     | 2.23                     | 0.46              |
| 4:QD:187:ARG:HH11  | 4:QD:187:ARG:HG2   | 1.81                     | 0.46              |
| 5:QE:12:LEU:HB3    | 5:QE:31:LEU:HB2    | 1.97                     | 0.46              |
| 7:QG:54:THR:O      | 7:QG:54:THR:HG23   | 2.16                     | 0.46              |
| 7:QG:57:GLU:O      | 7:QG:59:LEU:N      | 2.49                     | 0.46              |
| 8:QH:49:GLU:HG3    | 8:QH:49:GLU:O      | 2.15                     | 0.46              |
| 9:QI:80:GLY:C      | 9:QI:82:ALA:N      | 2.70                     | 0.46              |
| 13:QM:10:PRO:HG3   | 13:QM:18:ALA:O     | 2.16                     | 0.46              |
| 20:QT:44:ALA:O     | 20:QT:91:LEU:HB3   | 2.16                     | 0.46              |
| 20:QT:56:MET:HG3   | 20:QT:88:VAL:HG21  | 1.98                     | 0.46              |
| 25:RA:2233:U:H2'   | 25:RA:2234:G:C8    | 2.51                     | 0.46              |
| 25:RA:2349:G:OP2   | 54:R8:42:ARG:HD3   | 2.15                     | 0.46              |
| 27:RD:136:ILE:HD12 | 27:RD:136:ILE:N    | 2.30                     | 0.46              |
| 28:RE:50:GLY:CA    | 28:RE:74:PRO:HG3   | 2.46                     | 0.46              |
| 29:RF:111:ALA:O    | 29:RF:112:MET:C    | 2.59                     | 0.46              |
| 30:RG:37:VAL:HG22  | 30:RG:159:VAL:CA   | 2.34                     | 0.46              |
| 30:RG:44:GLY:C     | 30:RG:46:ALA:N     | 2.73                     | 0.46              |
| 30:RG:104:GLU:OE1  | 50:R4:23:GLU:HB3   | 2.15                     | 0.46              |
| 30:RG:111:LEU:HD22 | 30:RG:120:LEU:HD21 | 1.96                     | 0.46              |
| 31:RH:59:ARG:CG    | 31:RH:59:ARG:NH1   | 2.79                     | 0.46              |
| 33:RN:30:ILE:O     | 33:RN:34:LEU:CD2   | 2.64                     | 0.46              |
| 34:RO:86:ILE:H     | 34:RO:86:ILE:CD1   | 2.28                     | 0.46              |
| 35:RP:1:MET:O      | 35:RP:2:LYS:HG3    | 2.16                     | 0.46              |
| 39:RT:58:ASN:HD22  | 39:RT:58:ASN:N     | 2.10                     | 0.46              |
| 43:RX:43:VAL:HG11  | 43:RX:51:VAL:HG21  | 1.97                     | 0.46              |
| 45:RZ:104:PHE:CD1  | 45:RZ:139:VAL:HB   | 2.50                     | 0.46              |
| 46:R0:41:ARG:HA    | 46:R0:41:ARG:NE    | 2.31                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:881:G:P       | 12:XL:12:ARG:HH22  | 2.39                     | 0.46              |
| 1:XA:900:A:H2'     | 1:XA:901:A:C8      | 2.50                     | 0.46              |
| 1:XA:1414:U:H2'    | 1:XA:1415:G:H8     | 1.80                     | 0.46              |
| 2:XB:155:LEU:C     | 2:XB:157:ARG:H     | 2.23                     | 0.46              |
| 2:XB:162:ILE:CD1   | 2:XB:184:VAL:HG13  | 2.44                     | 0.46              |
| 4:XD:30:LYS:O      | 4:XD:32:ALA:N      | 2.49                     | 0.46              |
| 9:XI:42:ARG:O      | 9:XI:45:ALA:HB3    | 2.16                     | 0.46              |
| 10:XJ:4:ILE:O      | 10:XJ:74:ILE:HD13  | 2.16                     | 0.46              |
| 15:XO:82:ILE:HD11  | 15:XO:88:ARG:HG2   | 1.95                     | 0.46              |
| 18:XR:20:ALA:C     | 18:XR:21:LYS:HG3   | 2.41                     | 0.46              |
| 25:YA:1364:G:C8    | 47:Y1:2:SER:N      | 2.84                     | 0.46              |
| 25:YA:1426:G:OP2   | 25:YA:1427:A:O2'   | 2.28                     | 0.46              |
| 25:YA:2315:G:H2'   | 25:YA:2316:C:C6    | 2.51                     | 0.46              |
| 25:YA:2330:G:H2'   | 25:YA:2331:G:O4'   | 2.16                     | 0.46              |
| 25:YA:2345:G:OP2   | 52:Y6:39:TYR:CD2   | 2.69                     | 0.46              |
| 25:YA:2787:C:HO2'  | 25:YA:2810:A:HO2'  | 1.64                     | 0.46              |
| 27:YD:48:ARG:HG3   | 27:YD:48:ARG:NH1   | 2.31                     | 0.46              |
| 27:YD:79:VAL:HG21  | 27:YD:111:LEU:HD21 | 1.98                     | 0.46              |
| 27:YD:105:ILE:HG23 | 27:YD:106:ILE:O    | 2.15                     | 0.46              |
| 31:YH:88:LEU:HD22  | 31:YH:163:TYR:O    | 2.16                     | 0.46              |
| 31:YH:106:THR:HG22 | 31:YH:112:PRO:HB3  | 1.98                     | 0.46              |
| 33:YN:128:HIS:HB2  | 33:YN:129:PRO:CD   | 2.46                     | 0.46              |
| 35:YP:23:PRO:HG2   | 35:YP:23:PRO:O     | 2.15                     | 0.46              |
| 35:YP:36:LYS:HZ3   | 35:YP:36:LYS:HG3   | 1.39                     | 0.46              |
| 36:YQ:11:LYS:HE2   | 36:YQ:87:LYS:HA    | 1.98                     | 0.46              |
| 37:YR:75:LEU:HA    | 37:YR:78:LYS:HB3   | 1.98                     | 0.46              |
| 41:YV:22:VAL:HG12  | 41:YV:23:GLU:H     | 1.76                     | 0.46              |
| 42:YW:14:PRO:C     | 42:YW:16:LYS:N     | 2.73                     | 0.46              |
| 42:YW:14:PRO:C     | 42:YW:18:ARG:HD2   | 2.41                     | 0.46              |
| 44:YY:11:ASP:HB2   | 44:YY:27:VAL:CG1   | 2.46                     | 0.46              |
| 48:Y2:15:LYS:H     | 48:Y2:67:LYS:HZ3   | 1.64                     | 0.46              |
| 54:Y8:48:PHE:N     | 54:Y8:48:PHE:HD1   | 2.14                     | 0.46              |
| 1:QA:109:A:H2'     | 1:QA:326:G:N2      | 2.31                     | 0.46              |
| 1:QA:449:C:H5      | 16:QP:42:ARG:HH11  | 1.64                     | 0.46              |
| 1:QA:464:G:O6      | 1:QA:466:C:H5'     | 2.16                     | 0.46              |
| 1:QA:560:U:H4'     | 1:QA:561:U:O5'     | 2.16                     | 0.46              |
| 1:QA:690:G:H2'     | 1:QA:691:G:O4'     | 2.15                     | 0.46              |
| 2:QB:163:PHE:CE1   | 2:QB:215:LEU:HD22  | 2.50                     | 0.46              |
| 3:QC:42:LEU:HD12   | 3:QC:45:LYS:HZ3    | 1.81                     | 0.46              |
| 3:QC:68:VAL:HG12   | 3:QC:70:VAL:HG23   | 1.98                     | 0.46              |
| 4:QD:13:ARG:NH2    | 4:QD:36:ARG:NH2    | 2.64                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:QF:72:VAL:HG23  | 6:QF:90:VAL:HG11  | 1.98                     | 0.46              |
| 6:QF:101:ALA:HA   | 18:QR:28:GLU:CG   | 2.46                     | 0.46              |
| 8:QH:110:ALA:HB3  | 8:QH:121:ASP:HB3  | 1.98                     | 0.46              |
| 9:QI:71:SER:O     | 9:QI:72:GLY:C     | 2.58                     | 0.46              |
| 10:QJ:4:ILE:O     | 10:QJ:74:ILE:HD13 | 2.16                     | 0.46              |
| 11:QK:41:THR:CG2  | 11:QK:42:TRP:N    | 2.79                     | 0.46              |
| 11:QK:80:VAL:O    | 11:QK:106:LYS:HD3 | 2.15                     | 0.46              |
| 20:QT:98:PRO:O    | 20:QT:100:ILE:N   | 2.42                     | 0.46              |
| 25:RA:467:G:OP2   | 53:R7:34:ARG:NH1  | 2.46                     | 0.46              |
| 25:RA:1085:A:HO2' | 25:RA:1086:A:P    | 2.39                     | 0.46              |
| 25:RA:1936:A:H61  | 25:RA:1963:U:H3   | 1.64                     | 0.46              |
| 26:RB:50:G:OP1    | 38:RS:63:THR:HG23 | 2.16                     | 0.46              |
| 27:RD:45:ASN:CG   | 27:RD:46:GLN:N    | 2.68                     | 0.46              |
| 28:RE:7:VAL:HG11  | 39:RT:1:MET:CE    | 2.45                     | 0.46              |
| 30:RG:14:GLU:O    | 30:RG:17:PRO:HG2  | 2.15                     | 0.46              |
| 30:RG:88:ILE:O    | 30:RG:88:ILE:CD1  | 2.54                     | 0.46              |
| 31:RH:66:GLY:O    | 31:RH:67:LEU:C    | 2.58                     | 0.46              |
| 33:RN:36:GLY:O    | 33:RN:42:TRP:HE3  | 1.98                     | 0.46              |
| 33:RN:73:THR:HA   | 33:RN:83:LYS:O    | 2.15                     | 0.46              |
| 33:RN:112:LEU:O   | 33:RN:116:LEU:HG  | 2.16                     | 0.46              |
| 33:RN:114:ARG:C   | 33:RN:116:LEU:N   | 2.74                     | 0.46              |
| 34:RO:101:PRO:HA  | 34:RO:120:GLU:O   | 2.16                     | 0.46              |
| 35:RP:85:LEU:HD23 | 35:RP:88:LEU:HD22 | 1.97                     | 0.46              |
| 41:RV:67:GLY:O    | 41:RV:68:LYS:C    | 2.59                     | 0.46              |
| 47:R1:60:PHE:CE2  | 47:R1:91:LYS:NZ   | 2.84                     | 0.46              |
| 50:R4:4:GLY:O     | 50:R4:5:ILE:C     | 2.59                     | 0.46              |
| 51:R5:41:PRO:HA   | 51:R5:42:PRO:HD3  | 1.82                     | 0.46              |
| 1:XA:45:U:H2'     | 1:XA:46:G:H8      | 1.77                     | 0.46              |
| 1:XA:323:U:H2'    | 1:XA:324:G:O4'    | 2.16                     | 0.46              |
| 2:XB:75:LYS:C     | 2:XB:77:ALA:H     | 2.24                     | 0.46              |
| 2:XB:95:GLN:O     | 2:XB:96:ARG:C     | 2.59                     | 0.46              |
| 3:XC:46:GLU:C     | 3:XC:48:TYR:H     | 2.24                     | 0.46              |
| 3:XC:58:GLU:O     | 3:XC:59:ARG:HG3   | 2.15                     | 0.46              |
| 3:XC:78:GLY:HA3   | 3:XC:83:ARG:HB3   | 1.98                     | 0.46              |
| 9:XI:105:ASP:C    | 9:XI:107:ARG:N    | 2.74                     | 0.46              |
| 10:XJ:21:GLN:HG2  | 10:XJ:21:GLN:O    | 2.16                     | 0.46              |
| 10:XJ:32:ALA:HB3  | 10:XJ:76:ASN:CB   | 2.34                     | 0.46              |
| 15:XO:83:GLU:C    | 15:XO:85:LEU:N    | 2.71                     | 0.46              |
| 17:XQ:3:LYS:HD3   | 17:XQ:61:GLU:O    | 2.16                     | 0.46              |
| 25:YA:704:G:HO2'  | 25:YA:705:A:P     | 2.39                     | 0.46              |
| 25:YA:844:C:H2'   | 25:YA:845:G:O4'   | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1357:U:H2'   | 25:YA:1358:G:O4'   | 2.16                     | 0.46              |
| 25:YA:1407:C:H42   | 25:YA:1595:G:H1    | 1.63                     | 0.46              |
| 25:YA:1742:C:H5'   | 25:YA:1743:G:OP2   | 2.16                     | 0.46              |
| 27:YD:14:ARG:HG3   | 27:YD:15:PHE:N     | 2.31                     | 0.46              |
| 27:YD:35:LYS:HE3   | 27:YD:65:ILE:N     | 2.31                     | 0.46              |
| 27:YD:148:GLU:HB2  | 27:YD:151:LYS:HD2  | 1.98                     | 0.46              |
| 28:YE:1:MET:HA     | 28:YE:200:GLU:OE2  | 2.15                     | 0.46              |
| 28:YE:111:ARG:NE   | 28:YE:160:TYR:CE1  | 2.76                     | 0.46              |
| 30:YG:14:GLU:O     | 30:YG:17:PRO:HD2   | 2.16                     | 0.46              |
| 30:YG:83:ARG:HG3   | 30:YG:86:MET:CE    | 2.46                     | 0.46              |
| 33:YN:97:ARG:HA    | 33:YN:100:GLU:HB3  | 1.97                     | 0.46              |
| 34:YO:8:LEU:N      | 34:YO:8:LEU:CD2    | 2.76                     | 0.46              |
| 38:YS:61:ASN:O     | 38:YS:65:VAL:HG23  | 2.15                     | 0.46              |
| 42:YW:29:LEU:HD23  | 42:YW:29:LEU:C     | 2.41                     | 0.46              |
| 44:YY:15:VAL:O     | 44:YY:21:LYS:HA    | 2.16                     | 0.46              |
| 47:Y1:82:LEU:HD13  | 47:Y1:83:GLU:C     | 2.35                     | 0.46              |
| 49:Y3:43:ILE:O     | 49:Y3:47:VAL:HG23  | 2.16                     | 0.46              |
| 54:Y8:44:LYS:HD2   | 54:Y8:44:LYS:N     | 2.30                     | 0.46              |
| 1:QA:189:U:O2'     | 1:QA:190:G:OP1     | 2.33                     | 0.46              |
| 1:QA:793:U:H3'     | 1:QA:794:A:H5''    | 1.98                     | 0.46              |
| 1:QA:939:G:H1      | 1:QA:1344:C:N4     | 2.13                     | 0.46              |
| 1:QA:1200:C:H4'    | 1:QA:1201:A:H5''   | 1.97                     | 0.46              |
| 2:QB:77:ALA:HB1    | 2:QB:211:ILE:HG21  | 1.97                     | 0.46              |
| 4:QD:79:PHE:HE2    | 4:QD:83:SER:HB2    | 1.79                     | 0.46              |
| 5:QE:132:ALA:O     | 5:QE:133:TYR:C     | 2.59                     | 0.46              |
| 7:QG:103:TRP:O     | 7:QG:104:LEU:C     | 2.59                     | 0.46              |
| 9:QI:11:LYS:O      | 9:QI:12:GLU:HB2    | 2.16                     | 0.46              |
| 15:QO:30:ALA:HA    | 15:QO:85:LEU:HD11  | 1.97                     | 0.46              |
| 20:QT:22:ARG:O     | 20:QT:26:ASN:ND2   | 2.49                     | 0.46              |
| 20:QT:71:THR:HG22  | 20:QT:72:LEU:N     | 2.31                     | 0.46              |
| 21:QU:2:GLY:C      | 21:QU:4:GLY:H      | 2.23                     | 0.46              |
| 25:RA:994:C:H3'    | 40:RU:54:LYS:HE3   | 1.98                     | 0.46              |
| 25:RA:2119:A:C2    | 25:RA:2171:A:H1'   | 2.51                     | 0.46              |
| 25:RA:2518:A:H4'   | 25:RA:2519:U:OP1   | 2.16                     | 0.46              |
| 28:RE:47:VAL:O     | 28:RE:47:VAL:HG23  | 2.16                     | 0.46              |
| 28:RE:61:ARG:O     | 28:RE:63:LEU:CG    | 2.57                     | 0.46              |
| 28:RE:172:VAL:HG13 | 28:RE:182:LEU:HD11 | 1.98                     | 0.46              |
| 30:RG:14:GLU:O     | 30:RG:17:PRO:HD2   | 2.16                     | 0.46              |
| 30:RG:52:ILE:HG22  | 30:RG:52:ILE:O     | 2.15                     | 0.46              |
| 30:RG:135:LEU:HD11 | 30:RG:157:ILE:HD12 | 1.98                     | 0.46              |
| 31:RH:4:ILE:HG13   | 31:RH:6:ARG:HD3    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:RH:88:LEU:HD22 | 31:RH:163:TYR:O   | 2.16                     | 0.46              |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:CD  | 2.46                     | 0.46              |
| 34:RO:7:TYR:CD1   | 34:RO:20:MET:HB2  | 2.50                     | 0.46              |
| 35:RP:21:ARG:HB3  | 35:RP:22:GLY:H    | 1.65                     | 0.46              |
| 35:RP:23:PRO:HG2  | 35:RP:23:PRO:O    | 2.15                     | 0.46              |
| 37:RR:1:MET:O     | 37:RR:2:ARG:HB2   | 2.15                     | 0.46              |
| 38:RS:24:LEU:HB2  | 38:RS:85:VAL:HG12 | 1.98                     | 0.46              |
| 40:RU:27:LEU:HD12 | 40:RU:31:SER:HB3  | 1.98                     | 0.46              |
| 40:RU:69:CYS:O    | 40:RU:74:LEU:HD12 | 2.16                     | 0.46              |
| 42:RW:14:PRO:C    | 42:RW:18:ARG:HD2  | 2.41                     | 0.46              |
| 50:R4:23:GLU:O    | 50:R4:24:THR:OG1  | 2.34                     | 0.46              |
| 52:R6:7:ILE:O     | 52:R6:8:LYS:HG2   | 2.16                     | 0.46              |
| 54:R8:53:PRO:CD   | 54:R8:54:GLU:N    | 2.77                     | 0.46              |
| 1:XA:679:C:H2'    | 1:XA:680:C:C6     | 2.51                     | 0.46              |
| 1:XA:1446:A:H5'   | 39:YT:122:ASP:OD1 | 2.16                     | 0.46              |
| 2:XB:163:PHE:CE1  | 2:XB:215:LEU:HD22 | 2.50                     | 0.46              |
| 3:XC:53:ALA:O     | 3:XC:54:ARG:HB2   | 2.16                     | 0.46              |
| 3:XC:108:ASN:HB3  | 3:XC:111:LEU:HG   | 1.98                     | 0.46              |
| 7:XG:54:THR:O     | 7:XG:54:THR:HG23  | 2.16                     | 0.46              |
| 10:XJ:29:ARG:HG2  | 10:XJ:29:ARG:HH11 | 1.81                     | 0.46              |
| 10:XJ:44:VAL:HG12 | 10:XJ:45:ARG:N    | 2.30                     | 0.46              |
| 12:XL:11:VAL:HG21 | 17:XQ:34:LYS:HD3  | 1.96                     | 0.46              |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:N    | 2.30                     | 0.46              |
| 16:XP:40:ASP:O    | 16:XP:42:ARG:N    | 2.49                     | 0.46              |
| 19:XS:15:LEU:N    | 19:XS:15:LEU:CD2  | 2.79                     | 0.46              |
| 20:XT:22:ARG:O    | 20:XT:26:ASN:ND2  | 2.49                     | 0.46              |
| 25:YA:565:C:H2'   | 25:YA:566:U:O4'   | 2.16                     | 0.46              |
| 25:YA:855:G:H1    | 25:YA:922:U:H3    | 1.64                     | 0.46              |
| 25:YA:1266:G:C8   | 42:YW:15:ARG:NH1  | 2.84                     | 0.46              |
| 27:YD:2:ALA:HB1   | 27:YD:20:ASP:CB   | 2.46                     | 0.46              |
| 27:YD:36:PRO:HB3  | 27:YD:62:TYR:O    | 2.16                     | 0.46              |
| 28:YE:36:ARG:O    | 28:YE:37:ARG:C    | 2.59                     | 0.46              |
| 28:YE:87:GLU:O    | 28:YE:89:ASP:N    | 2.48                     | 0.46              |
| 28:YE:137:HIS:CB  | 28:YE:138:PRO:HD2 | 2.42                     | 0.46              |
| 30:YG:44:GLY:C    | 30:YG:46:ALA:N    | 2.73                     | 0.46              |
| 30:YG:129:GLY:O   | 30:YG:130:ASN:OD1 | 2.34                     | 0.46              |
| 33:YN:36:GLY:O    | 33:YN:42:TRP:CE3  | 2.69                     | 0.46              |
| 35:YP:85:LEU:HD23 | 35:YP:88:LEU:HD22 | 1.97                     | 0.46              |
| 36:YQ:87:LYS:O    | 36:YQ:87:LYS:HG2  | 2.15                     | 0.46              |
| 38:YS:108:GLY:O   | 38:YS:110:LEU:N   | 2.48                     | 0.46              |
| 39:YT:54:ARG:HG2  | 39:YT:54:ARG:NH1  | 2.23                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:YX:35:THR:O     | 43:YX:35:THR:HG23 | 2.16                     | 0.46              |
| 52:Y6:45:LYS:HD3   | 52:Y6:45:LYS:HA   | 1.79                     | 0.46              |
| 1:QA:1060:C:C5     | 3:QC:2:GLY:HA2    | 2.51                     | 0.46              |
| 1:QA:1521:G:H2'    | 1:QA:1522:U:H6    | 1.81                     | 0.46              |
| 2:QB:95:GLN:HA     | 2:QB:95:GLN:OE1   | 2.16                     | 0.46              |
| 3:QC:43:LEU:HD22   | 3:QC:47:LEU:CD2   | 2.46                     | 0.46              |
| 4:QD:29:PRO:CD     | 4:QD:30:LYS:H     | 2.29                     | 0.46              |
| 4:QD:72:GLU:O      | 4:QD:73:ARG:C     | 2.52                     | 0.46              |
| 4:QD:173:TRP:NE1   | 4:QD:174:LEU:HG   | 2.31                     | 0.46              |
| 6:QF:44:GLY:HA2    | 6:QF:59:TYR:CE2   | 2.51                     | 0.46              |
| 6:QF:69:GLU:O      | 6:QF:71:ARG:N     | 2.48                     | 0.46              |
| 6:QF:98:LEU:HD12   | 6:QF:98:LEU:C     | 2.41                     | 0.46              |
| 7:QG:107:ALA:O     | 7:QG:110:GLN:HB2  | 2.15                     | 0.46              |
| 10:QJ:96:ILE:N     | 10:QJ:96:ILE:CD1  | 2.79                     | 0.46              |
| 12:QL:27:LEU:HD13  | 12:QL:28:LYS:N    | 2.30                     | 0.46              |
| 13:QM:3:ARG:O      | 13:QM:4:ILE:HD13  | 2.17                     | 0.46              |
| 15:QO:74:ASP:C     | 15:QO:76:GLU:H    | 2.24                     | 0.46              |
| 16:QP:75:ARG:C     | 16:QP:77:ALA:N    | 2.72                     | 0.46              |
| 17:QQ:84:LEU:O     | 17:QQ:86:GLU:N    | 2.49                     | 0.46              |
| 17:QQ:100:LYS:O    | 17:QQ:101:ARG:HB2 | 2.15                     | 0.46              |
| 20:QT:93:GLU:HG2   | 20:QT:93:GLU:O    | 2.15                     | 0.46              |
| 22:QV:49:G:O6      | 22:QV:65:C:N4     | 2.49                     | 0.46              |
| 22:QV:56:C:HO2'    | 30:RG:78:SER:HB2  | 1.78                     | 0.46              |
| 25:RA:21:A:H2'     | 25:RA:22:C:C6     | 2.50                     | 0.46              |
| 25:RA:844:C:H2'    | 25:RA:845:G:O4'   | 2.16                     | 0.46              |
| 25:RA:1278:A:O3'   | 37:RR:34:ILE:HG23 | 2.16                     | 0.46              |
| 25:RA:1356:G:C6    | 25:RA:1357:U:C4   | 3.04                     | 0.46              |
| 25:RA:1851:U:H3    | 25:RA:1891:G:H1   | 1.64                     | 0.46              |
| 25:RA:2313:C:H4'   | 30:RG:40:ASN:OD1  | 2.16                     | 0.46              |
| 27:RD:35:LYS:HE3   | 27:RD:65:ILE:N    | 2.31                     | 0.46              |
| 27:RD:211:ARG:HH11 | 27:RD:211:ARG:HG2 | 1.80                     | 0.46              |
| 28:RE:1:MET:HE2    | 28:RE:1:MET:N     | 2.31                     | 0.46              |
| 30:RG:76:SER:CB    | 30:RG:83:ARG:HA   | 2.46                     | 0.46              |
| 31:RH:13:LYS:HE2   | 31:RH:13:LYS:CA   | 2.40                     | 0.46              |
| 31:RH:37:VAL:HG11  | 31:RH:68:THR:HG23 | 1.99                     | 0.46              |
| 32:RI:135:GLU:HB2  | 32:RI:136:VAL:H   | 1.65                     | 0.46              |
| 33:RN:17:ASP:O     | 33:RN:55:VAL:O    | 2.34                     | 0.46              |
| 35:RP:46:LYS:O     | 35:RP:48:PRO:N    | 2.48                     | 0.46              |
| 36:RQ:26:TYR:O     | 36:RQ:27:VAL:O    | 2.34                     | 0.46              |
| 36:RQ:27:VAL:HG22  | 36:RQ:105:GLU:CD  | 2.41                     | 0.46              |
| 48:R2:18:PRO:C     | 48:R2:20:GLU:N    | 2.73                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:R2:65:ASN:O    | 48:R2:66:GLU:C    | 2.59                     | 0.46              |
| 52:R6:15:GLU:OE2  | 52:R6:44:ARG:NH1  | 2.49                     | 0.46              |
| 1:XA:271:C:H2'    | 1:XA:272:C:H6     | 1.81                     | 0.46              |
| 1:XA:337:C:H2'    | 1:XA:338:A:C8     | 2.51                     | 0.46              |
| 1:XA:1200:C:H4'   | 1:XA:1201:A:C5'   | 2.46                     | 0.46              |
| 1:XA:1239:A:O2'   | 1:XA:1298:C:N4    | 2.49                     | 0.46              |
| 1:XA:1252:A:H2'   | 1:XA:1253:G:O4'   | 2.16                     | 0.46              |
| 1:XA:1432:G:H8    | 1:XA:1432:G:O5'   | 1.99                     | 0.46              |
| 2:XB:24:TRP:CZ2   | 2:XB:26:PRO:HB3   | 2.51                     | 0.46              |
| 3:XC:15:THR:HG22  | 3:XC:15:THR:O     | 2.15                     | 0.46              |
| 4:XD:52:SER:H     | 4:XD:55:ALA:HB3   | 1.81                     | 0.46              |
| 4:XD:92:VAL:O     | 4:XD:96:LEU:CD2   | 2.64                     | 0.46              |
| 4:XD:173:TRP:NE1  | 4:XD:174:LEU:HG   | 2.31                     | 0.46              |
| 7:XG:57:GLU:O     | 7:XG:59:LEU:N     | 2.49                     | 0.46              |
| 9:XI:11:LYS:O     | 9:XI:12:GLU:HB2   | 2.16                     | 0.46              |
| 11:XK:104:GLN:O   | 11:XK:106:LYS:HG3 | 2.16                     | 0.46              |
| 13:XM:10:PRO:HG3  | 13:XM:18:ALA:O    | 2.15                     | 0.46              |
| 15:XO:82:ILE:O    | 15:XO:86:GLY:N    | 2.49                     | 0.46              |
| 16:XP:19:ILE:HB   | 16:XP:37:GLY:O    | 2.16                     | 0.46              |
| 17:XQ:84:LEU:O    | 17:XQ:86:GLU:N    | 2.49                     | 0.46              |
| 20:XT:101:GLY:C   | 20:XT:103:GLY:N   | 2.73                     | 0.46              |
| 25:YA:861:A:H2'   | 25:YA:862:G:O4'   | 2.16                     | 0.46              |
| 25:YA:2562:U:H1'  | 34:YO:23:ARG:NH1  | 2.31                     | 0.46              |
| 25:YA:2695:C:H2'  | 25:YA:2696:U:H6   | 1.77                     | 0.46              |
| 27:YD:11:PRO:O    | 27:YD:12:SER:CB   | 2.64                     | 0.46              |
| 28:YE:54:GLN:HE21 | 28:YE:54:GLN:CA   | 2.27                     | 0.46              |
| 28:YE:94:GLU:C    | 28:YE:96:PHE:N    | 2.73                     | 0.46              |
| 29:YF:31:HIS:O    | 29:YF:34:TRP:HB3  | 2.15                     | 0.46              |
| 30:YG:76:SER:CB   | 30:YG:83:ARG:HA   | 2.46                     | 0.46              |
| 31:YH:128:PRO:HD2 | 31:YH:129:THR:N   | 2.25                     | 0.46              |
| 35:YP:98:GLU:HG2  | 35:YP:99:LEU:N    | 2.30                     | 0.46              |
| 38:YS:13:ARG:O    | 38:YS:14:VAL:HB   | 2.15                     | 0.46              |
| 44:YY:35:TYR:CD1  | 44:YY:35:TYR:O    | 2.69                     | 0.46              |
| 44:YY:49:VAL:O    | 44:YY:50:ARG:C    | 2.59                     | 0.46              |
| 47:Y1:79:GLY:N    | 47:Y1:80:LEU:HD23 | 2.30                     | 0.46              |
| 50:Y4:4:GLY:O     | 50:Y4:5:ILE:C     | 2.59                     | 0.46              |
| 52:Y6:11:LEU:HD11 | 52:Y6:51:GLU:HG3  | 1.98                     | 0.46              |
| 54:Y8:56:GLU:C    | 54:Y8:58:ILE:N    | 2.73                     | 0.46              |
| 1:QA:529:G:O6     | 12:QL:49:ASN:HA   | 2.16                     | 0.45              |
| 2:QB:30:ARG:O     | 2:QB:31:TYR:HD2   | 2.00                     | 0.45              |
| 3:QC:127:ARG:CG   | 3:QC:127:ARG:NH1  | 2.74                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:QD:100:ARG:NH2  | 4:QD:137:SER:HA    | 2.31                     | 0.45              |
| 4:QD:126:ILE:HG22 | 4:QD:127:THR:H     | 1.80                     | 0.45              |
| 4:QD:133:VAL:HG12 | 4:QD:135:LEU:H     | 1.81                     | 0.45              |
| 8:QH:91:ARG:HG2   | 8:QH:91:ARG:NH1    | 2.25                     | 0.45              |
| 9:QI:5:TYR:OH     | 9:QI:7:THR:HG23    | 2.15                     | 0.45              |
| 11:QK:121:PRO:HD2 | 11:QK:126:ARG:CD   | 2.46                     | 0.45              |
| 13:QM:8:GLU:C     | 13:QM:9:ILE:CG2    | 2.90                     | 0.45              |
| 13:QM:23:TYR:HB3  | 13:QM:67:GLU:HA    | 1.97                     | 0.45              |
| 16:QP:50:LYS:HD3  | 16:QP:50:LYS:C     | 2.41                     | 0.45              |
| 25:RA:389:G:N1    | 35:RP:71:VAL:HG12  | 2.30                     | 0.45              |
| 25:RA:896:A:H2    | 45:RZ:146:ILE:HD11 | 1.82                     | 0.45              |
| 25:RA:987:G:H2'   | 25:RA:988:A:O4'    | 2.16                     | 0.45              |
| 25:RA:1543:A:H2   | 25:RA:1545:A:C5    | 2.33                     | 0.45              |
| 25:RA:2498:C:O2'  | 25:RA:2499:C:H5'   | 2.17                     | 0.45              |
| 26:RB:38:C:N4     | 26:RB:44:G:H1      | 2.13                     | 0.45              |
| 27:RD:80:ALA:O    | 27:RD:113:VAL:HG13 | 2.16                     | 0.45              |
| 28:RE:15:PHE:CD1  | 28:RE:20:ALA:HB2   | 2.50                     | 0.45              |
| 31:RH:137:ASP:HB2 | 31:RH:140:LYS:HE3  | 1.98                     | 0.45              |
| 34:RO:61:VAL:O    | 34:RO:84:ALA:HB1   | 2.16                     | 0.45              |
| 35:RP:98:GLU:HG2  | 35:RP:99:LEU:N     | 2.30                     | 0.45              |
| 35:RP:115:LEU:CD1 | 35:RP:116:GLY:N    | 2.78                     | 0.45              |
| 36:RQ:104:PHE:O   | 36:RQ:105:GLU:CB   | 2.65                     | 0.45              |
| 38:RS:109:GLY:O   | 38:RS:110:LEU:HB2  | 2.16                     | 0.45              |
| 40:RU:106:PHE:O   | 40:RU:109:LEU:HB2  | 2.15                     | 0.45              |
| 43:RX:53:LYS:HZ2  | 43:RX:55:ASN:HD21  | 1.65                     | 0.45              |
| 44:RY:90:LEU:N    | 44:RY:90:LEU:CD2   | 2.73                     | 0.45              |
| 47:R1:85:LEU:N    | 47:R1:85:LEU:HD22  | 2.31                     | 0.45              |
| 49:R3:7:LYS:HE2   | 49:R3:32:GLN:HA    | 1.98                     | 0.45              |
| 1:XA:582:U:H2'    | 1:XA:583:A:C8      | 2.51                     | 0.45              |
| 1:XA:666:G:H5'    | 1:XA:726:C:H1'     | 1.99                     | 0.45              |
| 1:XA:974:A:N3     | 14:YN:31:ARG:NE    | 2.63                     | 0.45              |
| 2:XB:87:ARG:NH1   | 2:XB:220:ASP:OD1   | 2.46                     | 0.45              |
| 2:XB:109:SER:C    | 2:XB:111:ARG:N     | 2.73                     | 0.45              |
| 2:XB:214:ILE:HD13 | 2:XB:217:ARG:HH22  | 1.81                     | 0.45              |
| 3:XC:129:ALA:C    | 3:XC:131:ARG:N     | 2.72                     | 0.45              |
| 3:XC:172:ARG:O    | 3:XC:173:VAL:HG23  | 2.15                     | 0.45              |
| 4:XD:146:ILE:HG22 | 4:XD:146:ILE:O     | 2.15                     | 0.45              |
| 5:XE:12:LEU:HB3   | 5:XE:31:LEU:HB2    | 1.98                     | 0.45              |
| 6:XF:3:ARG:HH11   | 6:XF:3:ARG:HG3     | 1.80                     | 0.45              |
| 8:XH:33:GLU:O     | 8:XH:35:ILE:N      | 2.49                     | 0.45              |
| 8:XH:64:LYS:HB3   | 8:XH:79:VAL:HG21   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:XI:43:ALA:C     | 9:XI:45:ALA:N     | 2.73                     | 0.45              |
| 11:XK:41:THR:CG2  | 11:XK:42:TRP:N    | 2.79                     | 0.45              |
| 13:XM:3:ARG:O     | 13:XM:4:ILE:HD13  | 2.16                     | 0.45              |
| 13:XM:80:ARG:O    | 13:XM:82:MET:O    | 2.34                     | 0.45              |
| 19:XS:24:ALA:O    | 19:XS:25:LYS:CB   | 2.63                     | 0.45              |
| 25:YA:350:U:H2'   | 25:YA:351:G:O4'   | 2.16                     | 0.45              |
| 25:YA:1882:C:H5'  | 25:YA:1883:G:OP2  | 2.15                     | 0.45              |
| 25:YA:2168:G:H2'  | 25:YA:2168:G:N3   | 2.31                     | 0.45              |
| 25:YA:2401:U:H2'  | 25:YA:2402:C:H5'' | 1.98                     | 0.45              |
| 28:YE:101:ARG:C   | 28:YE:201:THR:OG1 | 2.58                     | 0.45              |
| 29:YF:65:TRP:CH2  | 29:YF:72:ARG:HB3  | 2.50                     | 0.45              |
| 30:YG:6:ALA:HB3   | 30:YG:104:GLU:OE2 | 2.16                     | 0.45              |
| 30:YG:14:GLU:HB3  | 30:YG:15:VAL:H    | 1.56                     | 0.45              |
| 30:YG:78:SER:O    | 30:YG:79:ASN:C    | 2.59                     | 0.45              |
| 35:YP:37:GLY:O    | 35:YP:38:GLN:C    | 2.58                     | 0.45              |
| 35:YP:115:LEU:HA  | 35:YP:134:ALA:CB  | 2.47                     | 0.45              |
| 36:YQ:27:VAL:HG22 | 36:YQ:105:GLU:CD  | 2.41                     | 0.45              |
| 41:YV:5:VAL:HG22  | 41:YV:14:VAL:CG2  | 2.46                     | 0.45              |
| 42:YW:14:PRO:O    | 42:YW:15:ARG:C    | 2.58                     | 0.45              |
| 45:YZ:10:ARG:HB2  | 45:YZ:38:TYR:HD2  | 1.79                     | 0.45              |
| 49:Y3:18:ASP:O    | 49:Y3:21:ALA:N    | 2.49                     | 0.45              |
| 50:Y4:3:GLU:HG3   | 50:Y4:4:GLY:H     | 1.79                     | 0.45              |
| 51:Y5:43:HIS:ND1  | 51:Y5:43:HIS:N    | 2.63                     | 0.45              |
| 55:Y9:1:MET:SD    | 55:Y9:31:LYS:O    | 2.74                     | 0.45              |
| 1:QA:380:G:C2     | 1:QA:384:G:C6     | 3.04                     | 0.45              |
| 1:QA:1509:C:H2'   | 1:QA:1510:U:O4'   | 2.16                     | 0.45              |
| 3:QC:46:GLU:C     | 3:QC:48:TYR:H     | 2.23                     | 0.45              |
| 3:QC:53:ALA:O     | 3:QC:54:ARG:HB2   | 2.16                     | 0.45              |
| 3:QC:172:ARG:O    | 3:QC:173:VAL:CG2  | 2.63                     | 0.45              |
| 4:QD:93:PHE:CZ    | 4:QD:97:LEU:HD11  | 2.52                     | 0.45              |
| 5:QE:64:ARG:HH11  | 5:QE:64:ARG:HG3   | 1.82                     | 0.45              |
| 5:QE:111:GLU:C    | 5:QE:113:ALA:N    | 2.73                     | 0.45              |
| 6:QF:75:LEU:HD23  | 6:QF:75:LEU:C     | 2.41                     | 0.45              |
| 8:QH:68:ARG:HH11  | 8:QH:68:ARG:HG2   | 1.81                     | 0.45              |
| 9:QI:105:ASP:C    | 9:QI:107:ARG:N    | 2.74                     | 0.45              |
| 12:QL:6:THR:H     | 12:QL:9:GLN:NE2   | 1.97                     | 0.45              |
| 12:QL:113:ARG:NH2 | 12:QL:120:TYR:CE2 | 2.85                     | 0.45              |
| 14:QN:26:ARG:NE   | 14:QN:47:LEU:HD21 | 2.30                     | 0.45              |
| 15:QO:5:LYS:O     | 15:QO:8:LYS:CG    | 2.63                     | 0.45              |
| 16:QP:40:ASP:O    | 16:QP:42:ARG:N    | 2.50                     | 0.45              |
| 17:QQ:86:GLU:O    | 17:QQ:87:LYS:C    | 2.60                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:566:U:OP1    | 35:RP:29:LYS:HE2   | 2.16                     | 0.45              |
| 25:RA:685:A:OP1    | 53:R7:11:LYS:NZ    | 2.45                     | 0.45              |
| 25:RA:1728:G:H5'   | 25:RA:1729:A:OP2   | 2.16                     | 0.45              |
| 26:RB:52:A:O2'     | 26:RB:53:A:N7      | 2.41                     | 0.45              |
| 27:RD:105:ILE:HG23 | 27:RD:106:ILE:O    | 2.15                     | 0.45              |
| 27:RD:154:LYS:C    | 27:RD:155:LEU:HD12 | 2.41                     | 0.45              |
| 30:RG:83:ARG:HG3   | 30:RG:86:MET:CE    | 2.46                     | 0.45              |
| 31:RH:89:ILE:H     | 31:RH:89:ILE:HD13  | 1.81                     | 0.45              |
| 31:RH:151:ILE:O    | 31:RH:152:ARG:O    | 2.34                     | 0.45              |
| 34:RO:104:ARG:HG2  | 34:RO:121:VAL:HG12 | 1.97                     | 0.45              |
| 35:RP:65:ARG:C     | 35:RP:66:GLY:O     | 2.59                     | 0.45              |
| 36:RQ:30:GLY:CA    | 36:RQ:107:ALA:HB2  | 2.39                     | 0.45              |
| 36:RQ:63:LYS:HE2   | 36:RQ:65:PHE:CZ    | 2.51                     | 0.45              |
| 36:RQ:85:LYS:HD3   | 36:RQ:86:GLY:H     | 1.81                     | 0.45              |
| 36:RQ:87:LYS:O     | 36:RQ:87:LYS:HG2   | 2.15                     | 0.45              |
| 37:RR:28:LEU:HD13  | 37:RR:28:LEU:C     | 2.40                     | 0.45              |
| 39:RT:24:PRO:HD3   | 39:RT:52:ILE:HD12  | 1.98                     | 0.45              |
| 40:RU:27:LEU:C     | 40:RU:29:SER:N     | 2.74                     | 0.45              |
| 40:RU:57:PHE:O     | 40:RU:59:ARG:N     | 2.50                     | 0.45              |
| 40:RU:79:PHE:CE2   | 40:RU:83:LEU:HD13  | 2.52                     | 0.45              |
| 44:RY:47:LYS:O     | 44:RY:49:VAL:N     | 2.48                     | 0.45              |
| 48:R2:48:HIS:O     | 48:R2:49:LYS:C     | 2.57                     | 0.45              |
| 49:R3:43:ILE:O     | 49:R3:47:VAL:HG23  | 2.15                     | 0.45              |
| 49:R3:60:GLU:HG2   | 49:R3:60:GLU:O     | 2.16                     | 0.45              |
| 50:R4:56:VAL:HA    | 50:R4:60:GLN:CB    | 2.28                     | 0.45              |
| 55:R9:25:VAL:HG11  | 55:R9:34:GLN:HE21  | 1.80                     | 0.45              |
| 1:XA:296:U:H2'     | 1:XA:297:G:C8      | 2.51                     | 0.45              |
| 1:XA:1053:G:H2'    | 1:XA:1199:U:C5     | 2.50                     | 0.45              |
| 1:XA:1291:G:H4'    | 9:XI:39:GLY:HA3    | 1.99                     | 0.45              |
| 2:XB:37:ASN:C      | 2:XB:39:ILE:N      | 2.74                     | 0.45              |
| 4:XD:192:GLU:H     | 4:XD:192:GLU:HG3   | 1.57                     | 0.45              |
| 4:XD:199:ASN:O     | 4:XD:201:GLN:N     | 2.50                     | 0.45              |
| 5:XE:42:GLY:CA     | 5:XE:136:MET:HE1   | 2.46                     | 0.45              |
| 5:XE:132:ALA:O     | 5:XE:133:TYR:C     | 2.59                     | 0.45              |
| 6:XF:100:ASN:HD22  | 6:XF:100:ASN:HA    | 1.48                     | 0.45              |
| 7:XG:95:ARG:NE     | 7:XG:99:LEU:HD11   | 2.30                     | 0.45              |
| 10:XJ:39:PRO:CB    | 10:XJ:70:ARG:HH12  | 2.27                     | 0.45              |
| 15:XO:5:LYS:O      | 15:XO:8:LYS:CG     | 2.63                     | 0.45              |
| 15:XO:30:ALA:HA    | 15:XO:85:LEU:HD11  | 1.97                     | 0.45              |
| 16:XP:71:ARG:HB2   | 16:XP:71:ARG:HH11  | 1.79                     | 0.45              |
| 17:XQ:86:GLU:O     | 17:XQ:87:LYS:C     | 2.60                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:YA:127:A:H5''    | 25:YA:128:C:C6     | 2.52                     | 0.45              |
| 25:YA:1061:U:H3'    | 25:YA:1062:G:H5''  | 1.97                     | 0.45              |
| 25:YA:1676:A:H2'    | 25:YA:1677:A:O4'   | 2.16                     | 0.45              |
| 25:YA:1998:G:OP2    | 28:YE:136:ARG:NH2  | 2.43                     | 0.45              |
| 25:YA:2072:G:H2'    | 25:YA:2073:C:H6    | 1.82                     | 0.45              |
| 25:YA:2126:A:H1'    | 25:YA:2127:G:OP2   | 2.16                     | 0.45              |
| 25:YA:2371:G:O2'    | 52:Y6:45:LYS:HB3   | 2.16                     | 0.45              |
| 27:YD:18:VAL:CG1    | 27:YD:19:ALA:N     | 2.78                     | 0.45              |
| 28:YE:62:PRO:O      | 28:YE:63:LEU:C     | 2.59                     | 0.45              |
| 28:YE:77:ILE:O      | 28:YE:78:LEU:O     | 2.35                     | 0.45              |
| 29:YF:167:ALA:HB1   | 29:YF:173:VAL:HG11 | 1.98                     | 0.45              |
| 31:YH:51:ARG:HG3    | 31:YH:51:ARG:NH1   | 2.30                     | 0.45              |
| 34:YO:86:ILE:H      | 34:YO:86:ILE:CD1   | 2.28                     | 0.45              |
| 35:YP:12:ALA:C      | 35:YP:14:LYS:N     | 2.73                     | 0.45              |
| 38:YS:102:ALA:C     | 38:YS:104:GLY:N    | 2.73                     | 0.45              |
| 39:YT:107:ASP:HB2   | 39:YT:108:ARG:H    | 1.48                     | 0.45              |
| 41:YV:47:VAL:O      | 41:YV:48:GLY:O     | 2.34                     | 0.45              |
| 43:YX:8:ILE:CD1     | 43:YX:42:ALA:HB1   | 2.46                     | 0.45              |
| 43:YX:53:LYS:HZ2    | 43:YX:55:ASN:HD21  | 1.63                     | 0.45              |
| 45:YZ:95:PRO:HB2    | 45:YZ:127:LYS:HG2  | 1.97                     | 0.45              |
| 47:Y1:49:VAL:HG12   | 47:Y1:51:VAL:CG2   | 2.45                     | 0.45              |
| 49:Y3:7:LYS:HE2     | 49:Y3:32:GLN:HA    | 1.98                     | 0.45              |
| 51:Y5:16:ARG:O      | 51:Y5:20:ARG:HG3   | 2.16                     | 0.45              |
| 52:Y6:17:LYS:O      | 52:Y6:18:ARG:CB    | 2.64                     | 0.45              |
| 1:QA:59:A:H3'       | 1:QA:331:G:H22     | 1.81                     | 0.45              |
| 1:QA:372:C:H2'      | 1:QA:372:C:O2      | 2.16                     | 0.45              |
| 1:QA:1053:G:H5'     | 1:QA:1054:C:H5'    | 1.98                     | 0.45              |
| 2:QB:22:LYS:O       | 2:QB:24:TRP:N      | 2.50                     | 0.45              |
| 2:QB:24:TRP:CZ2     | 2:QB:26:PRO:HB3    | 2.51                     | 0.45              |
| 3:QC:92:ALA:HB2     | 3:QC:99:VAL:HG11   | 1.98                     | 0.45              |
| 3:QC:108:ASN:CG     | 3:QC:111:LEU:HG    | 2.41                     | 0.45              |
| 4:QD:52:SER:H       | 4:QD:55:ALA:HB3    | 1.82                     | 0.45              |
| 4:QD:92:VAL:O       | 4:QD:96:LEU:CD2    | 2.64                     | 0.45              |
| 8:QH:33:GLU:O       | 8:QH:35:ILE:N      | 2.49                     | 0.45              |
| 19:QS:10:PHE:CD1    | 19:QS:38:SER:HB2   | 2.52                     | 0.45              |
| 25:RA:207:A:H2'     | 25:RA:208:C:O4'    | 2.15                     | 0.45              |
| 25:RA:270(B):A:N7   | 25:RA:270(X):G:N2  | 2.63                     | 0.45              |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:CD2   | 2.32                     | 0.45              |
| 25:RA:831:G:H2'     | 25:RA:832:G:O4'    | 2.17                     | 0.45              |
| 25:RA:942:G:O2'     | 25:RA:1189:A:N3    | 2.40                     | 0.45              |
| 25:RA:1047:G:H2'    | 25:RA:1110:G:H1    | 1.81                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1534:G:N3   | 25:RA:1534:G:H2'   | 2.32                     | 0.45              |
| 25:RA:2012:G:H4'  | 42:RW:96:ILE:HD11  | 1.98                     | 0.45              |
| 25:RA:2350:C:H5   | 54:R8:42:ARG:NH1   | 2.15                     | 0.45              |
| 25:RA:2354:G:O2'  | 46:R0:36:ILE:HG23  | 2.16                     | 0.45              |
| 27:RD:145:VAL:HB  | 27:RD:155:LEU:HB2  | 1.99                     | 0.45              |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:CD    | 2.46                     | 0.45              |
| 33:RN:22:THR:O    | 33:RN:60:ILE:HG22  | 2.16                     | 0.45              |
| 36:RQ:52:VAL:O    | 36:RQ:53:ALA:C     | 2.59                     | 0.45              |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:N     | 2.32                     | 0.45              |
| 39:RT:36:GLU:CG   | 39:RT:41:ARG:HD3   | 2.46                     | 0.45              |
| 42:RW:29:LEU:HD23 | 42:RW:29:LEU:C     | 2.41                     | 0.45              |
| 44:RY:75:ILE:HA   | 44:RY:80:GLY:HA2   | 1.99                     | 0.45              |
| 44:RY:81:LYS:CD   | 44:RY:97:ARG:HE    | 2.20                     | 0.45              |
| 4:XD:100:ARG:NH2  | 4:XD:137:SER:HA    | 2.32                     | 0.45              |
| 5:XE:7:GLU:HB3    | 5:XE:112:LEU:HD13  | 1.99                     | 0.45              |
| 5:XE:153:LYS:HD3  | 5:XE:153:LYS:C     | 2.41                     | 0.45              |
| 6:XF:44:GLY:HA2   | 6:XF:59:TYR:CE2    | 2.51                     | 0.45              |
| 6:XF:62:TRP:C     | 6:XF:63:TYR:CD2    | 2.92                     | 0.45              |
| 7:XG:95:ARG:HG2   | 7:XG:99:LEU:HD12   | 1.98                     | 0.45              |
| 10:XJ:95:GLU:OE2  | 10:XJ:95:GLU:HA    | 2.16                     | 0.45              |
| 12:XL:115:LYS:O   | 12:XL:117:ARG:N    | 2.47                     | 0.45              |
| 13:XM:65:LYS:NZ   | 13:XM:69:GLU:HG2   | 2.30                     | 0.45              |
| 18:XR:32:ARG:HH11 | 18:XR:65:ILE:HD13  | 1.80                     | 0.45              |
| 20:XT:96:GLY:O    | 20:XT:97:ALA:CB    | 2.64                     | 0.45              |
| 25:YA:769:G:H5'   | 25:YA:1379:A:N6    | 2.31                     | 0.45              |
| 25:YA:1317:A:H2'  | 25:YA:1318:C:H6    | 1.81                     | 0.45              |
| 25:YA:1728:G:H3'  | 25:YA:1729:A:H5''  | 1.98                     | 0.45              |
| 27:YD:65:ILE:HD11 | 27:YD:67:PHE:CE1   | 2.51                     | 0.45              |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:HD2  | 1.81                     | 0.45              |
| 27:YD:118:VAL:O   | 27:YD:129:ASN:HA   | 2.16                     | 0.45              |
| 28:YE:1:MET:N     | 28:YE:1:MET:HE2    | 2.31                     | 0.45              |
| 29:YF:7:TYR:CD1   | 29:YF:7:TYR:N      | 2.85                     | 0.45              |
| 29:YF:117:ARG:NH2 | 29:YF:189:THR:O    | 2.50                     | 0.45              |
| 30:YG:44:GLY:HA2  | 30:YG:88:ILE:HG12  | 1.97                     | 0.45              |
| 31:YH:16:SER:OG   | 31:YH:17:VAL:N     | 2.50                     | 0.45              |
| 31:YH:109:PHE:CE1 | 31:YH:152:ARG:NH1  | 2.85                     | 0.45              |
| 32:YI:77:LEU:HD11 | 32:YI:140:LEU:HD12 | 1.98                     | 0.45              |
| 33:YN:113:GLY:O   | 33:YN:116:LEU:HB2  | 2.14                     | 0.45              |
| 33:YN:114:ARG:O   | 33:YN:115:ARG:CB   | 2.65                     | 0.45              |
| 34:YO:112:MET:O   | 34:YO:115:VAL:CG2  | 2.64                     | 0.45              |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:HA2  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:YS:109:GLY:O   | 38:YS:110:LEU:HB2 | 2.16                     | 0.45              |
| 39:YT:10:VAL:O    | 39:YT:11:GLU:C    | 2.59                     | 0.45              |
| 41:YV:4:ILE:HG22  | 41:YV:39:LEU:HD23 | 1.98                     | 0.45              |
| 43:YX:54:VAL:C    | 43:YX:55:ASN:HD22 | 2.24                     | 0.45              |
| 44:YY:48:ALA:CB   | 44:YY:61:ILE:HD13 | 2.45                     | 0.45              |
| 48:Y2:18:PRO:C    | 48:Y2:20:GLU:N    | 2.73                     | 0.45              |
| 50:Y4:64:GLY:C    | 50:Y4:66:SER:N    | 2.73                     | 0.45              |
| 55:Y9:25:VAL:HG11 | 55:Y9:34:GLN:HE21 | 1.81                     | 0.45              |
| 1:QA:186:C:H5'    | 20:QT:78:ALA:HB1  | 1.98                     | 0.45              |
| 1:QA:191(E):G:H2' | 1:QA:191(F):U:C6  | 2.51                     | 0.45              |
| 2:QB:95:GLN:O     | 2:QB:96:ARG:C     | 2.59                     | 0.45              |
| 3:QC:108:ASN:HB3  | 3:QC:111:LEU:HD12 | 1.98                     | 0.45              |
| 4:QD:52:SER:N     | 4:QD:55:ALA:HB3   | 2.32                     | 0.45              |
| 4:QD:150:GLU:C    | 4:QD:152:SER:N    | 2.73                     | 0.45              |
| 5:QE:52:PRO:HB2   | 5:QE:53:LEU:HD12  | 1.97                     | 0.45              |
| 5:QE:72:GLN:C     | 5:QE:74:GLY:H     | 2.23                     | 0.45              |
| 5:QE:78:HIS:CD2   | 8:QH:104:ARG:CG   | 2.94                     | 0.45              |
| 6:QF:40:VAL:HG22  | 6:QF:41:GLU:H     | 1.80                     | 0.45              |
| 7:QG:50:ILE:HG21  | 7:QG:61:VAL:HG21  | 1.97                     | 0.45              |
| 8:QH:33:GLU:C     | 8:QH:35:ILE:H     | 2.25                     | 0.45              |
| 12:QL:64:TYR:O    | 12:QL:65:GLU:HB2  | 2.16                     | 0.45              |
| 13:QM:66:LEU:HB2  | 13:QM:67:GLU:H    | 1.61                     | 0.45              |
| 15:QO:11:VAL:O    | 15:QO:12:ILE:C    | 2.60                     | 0.45              |
| 15:QO:82:ILE:HD11 | 15:QO:88:ARG:HG2  | 1.95                     | 0.45              |
| 16:QP:19:ILE:HB   | 16:QP:37:GLY:O    | 2.16                     | 0.45              |
| 20:QT:47:GLY:C    | 20:QT:49:ALA:N    | 2.72                     | 0.45              |
| 25:RA:451:C:H4'   | 29:RF:52:LYS:NZ   | 2.32                     | 0.45              |
| 25:RA:1022:G:O2'  | 25:RA:1023:U:OP2  | 2.26                     | 0.45              |
| 25:RA:1354:A:OP1  | 27:RD:38:LYS:HE2  | 2.17                     | 0.45              |
| 25:RA:2015:A:N3   | 51:R5:2:ALA:N     | 2.65                     | 0.45              |
| 26:RB:15:A:H5'    | 26:RB:16:G:C8     | 2.51                     | 0.45              |
| 27:RD:2:ALA:HB1   | 27:RD:20:ASP:CB   | 2.46                     | 0.45              |
| 27:RD:148:GLU:HB2 | 27:RD:151:LYS:HD2 | 1.98                     | 0.45              |
| 28:RE:1:MET:HA    | 28:RE:200:GLU:OE2 | 2.16                     | 0.45              |
| 31:RH:94:TYR:N    | 31:RH:94:TYR:CD1  | 2.82                     | 0.45              |
| 34:RO:31:LYS:C    | 34:RO:32:TYR:CD2  | 2.94                     | 0.45              |
| 36:RQ:5:ARG:O     | 36:RQ:6:ARG:O     | 2.35                     | 0.45              |
| 38:RS:5:THR:OG1   | 38:RS:8:GLU:HG3   | 2.17                     | 0.45              |
| 39:RT:6:LEU:O     | 39:RT:10:VAL:HG23 | 2.16                     | 0.45              |
| 44:RY:36:ALA:HB1  | 44:RY:67:LEU:O    | 2.16                     | 0.45              |
| 50:R4:26:SER:C    | 50:R4:27:THR:O    | 2.58                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:R6:20:ASN:O    | 52:R6:21:TYR:HB2  | 2.15                     | 0.45              |
| 1:XA:272:C:H2'    | 1:XA:273:A:C8     | 2.52                     | 0.45              |
| 1:XA:336:C:H2'    | 1:XA:337:C:C6     | 2.52                     | 0.45              |
| 1:XA:1213:A:N1    | 1:XA:1215:G:H1'   | 2.31                     | 0.45              |
| 2:XB:25:ASN:HA    | 2:XB:26:PRO:HD2   | 1.86                     | 0.45              |
| 3:XC:43:LEU:HD22  | 3:XC:47:LEU:CD2   | 2.46                     | 0.45              |
| 4:XD:104:VAL:O    | 4:XD:107:ARG:N    | 2.49                     | 0.45              |
| 5:XE:90:VAL:C     | 5:XE:91:LEU:HD12  | 2.42                     | 0.45              |
| 7:XG:79:ARG:HG2   | 7:XG:79:ARG:NH1   | 2.29                     | 0.45              |
| 8:XH:33:GLU:C     | 8:XH:35:ILE:H     | 2.25                     | 0.45              |
| 11:XK:32:ILE:HD11 | 11:XK:72:ALA:HB2  | 1.95                     | 0.45              |
| 12:XL:64:TYR:O    | 12:XL:65:GLU:HB2  | 2.16                     | 0.45              |
| 13:XM:57:ARG:HD2  | 13:XM:61:GLU:OE2  | 2.17                     | 0.45              |
| 14:XN:43:CYS:HB3  | 14:XN:44:LEU:H    | 1.66                     | 0.45              |
| 15:XO:77:ARG:HA   | 15:XO:80:ALA:HB2  | 1.99                     | 0.45              |
| 20:XT:24:LEU:O    | 20:XT:24:LEU:HD13 | 2.16                     | 0.45              |
| 20:XT:26:ASN:ND2  | 20:XT:26:ASN:N    | 2.62                     | 0.45              |
| 25:YA:210:C:OP2   | 53:Y7:29:LYS:NZ   | 2.49                     | 0.45              |
| 25:YA:605:C:H1'   | 25:YA:657:U:O2'   | 2.15                     | 0.45              |
| 25:YA:888:C:H3'   | 25:YA:889:C:C4'   | 2.46                     | 0.45              |
| 25:YA:1021:A:H2'  | 25:YA:1023:U:H5'  | 1.98                     | 0.45              |
| 27:YD:109:ASP:HB2 | 27:YD:197:GLY:CA  | 2.46                     | 0.45              |
| 28:YE:13:ARG:HH11 | 28:YE:13:ARG:HB3  | 1.82                     | 0.45              |
| 28:YE:33:VAL:HG12 | 28:YE:90:THR:H    | 1.81                     | 0.45              |
| 36:YQ:85:LYS:HD3  | 36:YQ:86:GLY:H    | 1.81                     | 0.45              |
| 36:YQ:104:PHE:O   | 36:YQ:105:GLU:CB  | 2.65                     | 0.45              |
| 38:YS:5:THR:OG1   | 38:YS:8:GLU:HG3   | 2.17                     | 0.45              |
| 40:YU:5:LYS:C     | 40:YU:7:GLY:N     | 2.74                     | 0.45              |
| 40:YU:57:PHE:O    | 40:YU:58:ARG:C    | 2.59                     | 0.45              |
| 41:YV:30:GLY:O    | 41:YV:31:ALA:O    | 2.33                     | 0.45              |
| 43:YX:24:GLY:O    | 43:YX:82:GLN:HA   | 2.16                     | 0.45              |
| 47:Y1:54:ALA:O    | 47:Y1:55:GLY:O    | 2.35                     | 0.45              |
| 47:Y1:85:LEU:N    | 47:Y1:85:LEU:HD22 | 2.31                     | 0.45              |
| 52:Y6:9:LEU:CD1   | 52:Y6:26:ASN:ND2  | 2.79                     | 0.45              |
| 52:Y6:11:LEU:H    | 52:Y6:25:LYS:HA   | 1.81                     | 0.45              |
| 1:QA:596:C:H42    | 1:QA:644:G:H1     | 1.65                     | 0.45              |
| 1:QA:909:A:H2'    | 1:QA:910:C:O4'    | 2.17                     | 0.45              |
| 1:QA:1064:G:O2'   | 1:QA:1065:U:O5'   | 2.29                     | 0.45              |
| 2:QB:15:VAL:HG23  | 2:QB:209:ARG:HE   | 1.80                     | 0.45              |
| 2:QB:195:ASP:O    | 8:QH:68:ARG:NH2   | 2.50                     | 0.45              |
| 4:QD:29:PRO:HD2   | 4:QD:30:LYS:H     | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:QI:42:ARG:O      | 9:QI:45:ALA:HB3    | 2.16                     | 0.45              |
| 16:QP:58:TYR:O     | 16:QP:61:SER:OG    | 2.27                     | 0.45              |
| 25:RA:389:G:H22    | 35:RP:72:PRO:CG    | 2.29                     | 0.45              |
| 25:RA:492:A:H2'    | 25:RA:493:G:O4'    | 2.16                     | 0.45              |
| 25:RA:888:C:O2'    | 25:RA:889:C:H4'    | 2.15                     | 0.45              |
| 25:RA:2054:A:H5''  | 25:RA:2055:C:O5'   | 2.15                     | 0.45              |
| 27:RD:35:LYS:CE    | 27:RD:64:ILE:C     | 2.89                     | 0.45              |
| 27:RD:65:ILE:HD11  | 27:RD:67:PHE:CE1   | 2.51                     | 0.45              |
| 28:RE:22:PRO:O     | 28:RE:22:PRO:CG    | 2.63                     | 0.45              |
| 28:RE:62:PRO:O     | 28:RE:63:LEU:C     | 2.59                     | 0.45              |
| 30:RG:14:GLU:HB3   | 30:RG:15:VAL:H     | 1.56                     | 0.45              |
| 30:RG:51:ARG:NH2   | 30:RG:52:ILE:HD11  | 2.32                     | 0.45              |
| 31:RH:6:ARG:C      | 31:RH:8:PRO:CD     | 2.89                     | 0.45              |
| 31:RH:106:THR:HG22 | 31:RH:112:PRO:HB3  | 1.97                     | 0.45              |
| 31:RH:109:PHE:CE1  | 31:RH:152:ARG:NH1  | 2.85                     | 0.45              |
| 33:RN:5:VAL:O      | 33:RN:5:VAL:HG13   | 2.16                     | 0.45              |
| 33:RN:128:HIS:HB2  | 33:RN:129:PRO:CD   | 2.46                     | 0.45              |
| 34:RO:47:ILE:HG13  | 34:RO:48:PRO:HD2   | 1.99                     | 0.45              |
| 35:RP:21:ARG:HE    | 35:RP:21:ARG:HA    | 1.82                     | 0.45              |
| 35:RP:92:GLU:HA    | 35:RP:123:LEU:HD23 | 1.98                     | 0.45              |
| 36:RQ:93:TYR:CD1   | 36:RQ:93:TYR:N     | 2.85                     | 0.45              |
| 37:RR:10:LEU:C     | 37:RR:12:ARG:N     | 2.72                     | 0.45              |
| 42:RW:14:PRO:C     | 42:RW:16:LYS:N     | 2.73                     | 0.45              |
| 44:RY:57:GLN:O     | 44:RY:58:GLY:C     | 2.60                     | 0.45              |
| 51:R5:16:ARG:O     | 51:R5:20:ARG:HG3   | 2.16                     | 0.45              |
| 54:R8:40:GLU:C     | 54:R8:42:ARG:N     | 2.68                     | 0.45              |
| 54:R8:48:PHE:N     | 54:R8:48:PHE:HD1   | 2.14                     | 0.45              |
| 1:XA:347:G:C4      | 1:XA:348:G:C8      | 3.04                     | 0.45              |
| 1:XA:1002:G:H2'    | 1:XA:1003:G:C8     | 2.48                     | 0.45              |
| 1:XA:1072:G:C5     | 1:XA:1073:U:C4     | 3.04                     | 0.45              |
| 1:XA:1222:G:P      | 19:XS:77:THR:HG21  | 2.57                     | 0.45              |
| 2:XB:51:LEU:O      | 2:XB:55:PHE:HD2    | 2.00                     | 0.45              |
| 2:XB:95:GLN:OE1    | 2:XB:95:GLN:HA     | 2.16                     | 0.45              |
| 2:XB:240:GLN:HG2   | 2:XB:240:GLN:O     | 2.16                     | 0.45              |
| 3:XC:42:LEU:HD12   | 3:XC:45:LYS:NZ     | 2.32                     | 0.45              |
| 4:XD:52:SER:N      | 4:XD:55:ALA:HB3    | 2.32                     | 0.45              |
| 4:XD:133:VAL:HG12  | 4:XD:135:LEU:H     | 1.82                     | 0.45              |
| 5:XE:55:VAL:O      | 5:XE:58:ALA:HB3    | 2.16                     | 0.45              |
| 7:XG:103:TRP:O     | 7:XG:104:LEU:C     | 2.58                     | 0.45              |
| 7:XG:107:ALA:O     | 7:XG:110:GLN:HB2   | 2.15                     | 0.45              |
| 11:XK:48:ILE:HD11  | 11:XK:64:ALA:N     | 2.32                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:XN:43:CYS:C    | 14:XN:45:ARG:N     | 2.73                     | 0.45              |
| 15:XO:11:VAL:O    | 15:XO:12:ILE:C     | 2.60                     | 0.45              |
| 20:XT:53:LEU:HD12 | 20:XT:100:ILE:HG23 | 1.98                     | 0.45              |
| 25:YA:921:G:H4'   | 25:YA:2269:A:C5    | 2.52                     | 0.45              |
| 25:YA:1607:C:H4'  | 25:YA:1608:A:O5'   | 2.17                     | 0.45              |
| 25:YA:1669:A:C2   | 25:YA:1994:C:H1'   | 2.51                     | 0.45              |
| 25:YA:2335:A:HO2' | 25:YA:2336:A:P     | 2.39                     | 0.45              |
| 25:YA:2572:A:C4   | 28:YE:144:ARG:NH2  | 2.84                     | 0.45              |
| 25:YA:2584:U:H2'  | 25:YA:2585:U:H2'   | 1.98                     | 0.45              |
| 28:YE:51:PHE:HD1  | 28:YE:52:LEU:H     | 1.59                     | 0.45              |
| 30:YG:51:ARG:NH2  | 30:YG:52:ILE:HD11  | 2.32                     | 0.45              |
| 31:YH:66:GLY:O    | 31:YH:67:LEU:C     | 2.58                     | 0.45              |
| 36:YQ:26:TYR:O    | 36:YQ:27:VAL:O     | 2.34                     | 0.45              |
| 44:YY:75:ILE:HA   | 44:YY:80:GLY:HA2   | 1.99                     | 0.45              |
| 47:Y1:60:PHE:CE2  | 47:Y1:91:LYS:NZ    | 2.84                     | 0.45              |
| 48:Y2:65:ASN:O    | 48:Y2:66:GLU:C     | 2.59                     | 0.45              |
| 53:Y7:24:THR:O    | 53:Y7:28:ARG:HG3   | 2.16                     | 0.45              |
| 1:QA:973:G:O6     | 1:QA:974:A:N6      | 2.48                     | 0.45              |
| 2:QB:24:TRP:CD2   | 2:QB:26:PRO:HD3    | 2.52                     | 0.45              |
| 2:QB:33:TYR:HD1   | 2:QB:33:TYR:O      | 2.00                     | 0.45              |
| 3:QC:134:ILE:HG23 | 3:QC:151:VAL:HB    | 1.98                     | 0.45              |
| 4:QD:101:LEU:HD21 | 4:QD:121:VAL:HG13  | 1.98                     | 0.45              |
| 4:QD:104:VAL:O    | 4:QD:107:ARG:N     | 2.49                     | 0.45              |
| 4:QD:114:ARG:NH1  | 4:QD:114:ARG:CG    | 2.77                     | 0.45              |
| 5:QE:48:ALA:C     | 5:QE:50:GLU:H      | 2.24                     | 0.45              |
| 7:QG:95:ARG:HG2   | 7:QG:99:LEU:HD12   | 1.98                     | 0.45              |
| 8:QH:41:ARG:CG    | 8:QH:41:ARG:NH1    | 2.76                     | 0.45              |
| 8:QH:97:VAL:CG1   | 8:QH:98:LYS:H      | 2.30                     | 0.45              |
| 12:QL:61:THR:O    | 12:QL:63:GLY:N     | 2.45                     | 0.45              |
| 16:QP:50:LYS:HD3  | 16:QP:50:LYS:O     | 2.16                     | 0.45              |
| 20:QT:96:GLY:O    | 20:QT:99:LEU:HD13  | 2.16                     | 0.45              |
| 25:RA:49:A:H61    | 25:RA:177:G:H2'    | 1.82                     | 0.45              |
| 25:RA:997:G:OP1   | 40:RU:93:LYS:HD3   | 2.17                     | 0.45              |
| 25:RA:1079:C:O4'  | 25:RA:1088:A:N6    | 2.49                     | 0.45              |
| 25:RA:1152:C:H2'  | 25:RA:1153:C:C6    | 2.51                     | 0.45              |
| 25:RA:1508:A:O2'  | 25:RA:1509:C:O4'   | 2.33                     | 0.45              |
| 25:RA:2124:G:C2   | 25:RA:2125:G:H1'   | 2.52                     | 0.45              |
| 25:RA:2410:G:C2   | 25:RA:2411:A:H1'   | 2.51                     | 0.45              |
| 30:RG:20:ILE:HD13 | 30:RG:25:TYR:HB2   | 1.98                     | 0.45              |
| 31:RH:86:GLU:O    | 31:RH:87:LEU:CB    | 2.64                     | 0.45              |
| 33:RN:28:THR:O    | 33:RN:29:LYS:C     | 2.59                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:RN:35:ARG:HG3  | 33:RN:35:ARG:O    | 2.16                     | 0.45              |
| 33:RN:96:GLU:O    | 33:RN:99:LEU:N    | 2.34                     | 0.45              |
| 34:RO:40:VAL:CG1  | 34:RO:41:ALA:N    | 2.80                     | 0.45              |
| 35:RP:62:LEU:CD2  | 35:RP:62:LEU:H    | 2.19                     | 0.45              |
| 35:RP:88:LEU:O    | 35:RP:90:ARG:N    | 2.50                     | 0.45              |
| 39:RT:10:VAL:O    | 39:RT:11:GLU:C    | 2.59                     | 0.45              |
| 40:RU:73:GLY:O    | 40:RU:74:LEU:CB   | 2.63                     | 0.45              |
| 44:RY:49:VAL:O    | 44:RY:50:ARG:C    | 2.59                     | 0.45              |
| 45:RZ:69:THR:HG22 | 45:RZ:90:VAL:HG13 | 1.98                     | 0.45              |
| 48:R2:28:LYS:HB3  | 48:R2:57:ILE:HG12 | 1.97                     | 0.45              |
| 49:R3:28:LEU:HA   | 49:R3:33:GLN:OE1  | 2.16                     | 0.45              |
| 51:R5:15:ARG:HA   | 51:R5:18:ALA:HB3  | 1.99                     | 0.45              |
| 52:R6:11:LEU:H    | 52:R6:25:LYS:HA   | 1.81                     | 0.45              |
| 1:XA:240:C:H2'    | 1:XA:241:C:C6     | 2.51                     | 0.45              |
| 1:XA:753:A:H4'    | 1:XA:754:C:O5'    | 2.16                     | 0.45              |
| 1:XA:1000:A:H2'   | 1:XA:1001:G:H8    | 1.82                     | 0.45              |
| 1:XA:1218:C:H2'   | 1:XA:1219:U:H6    | 1.81                     | 0.45              |
| 1:XA:1321:C:C4    | 1:XA:1322:C:C4    | 3.04                     | 0.45              |
| 2:XB:77:ALA:HB2   | 2:XB:211:ILE:HG21 | 1.99                     | 0.45              |
| 2:XB:95:GLN:NE2   | 2:XB:96:ARG:NH1   | 2.65                     | 0.45              |
| 2:XB:170:GLU:CA   | 2:XB:172:ILE:HD12 | 2.46                     | 0.45              |
| 3:XC:22:TRP:HB3   | 3:XC:59:ARG:HB2   | 1.99                     | 0.45              |
| 4:XD:178:VAL:O    | 4:XD:181:MET:N    | 2.50                     | 0.45              |
| 4:XD:187:ARG:HH11 | 4:XD:187:ARG:HG2  | 1.82                     | 0.45              |
| 5:XE:12:LEU:HB3   | 5:XE:31:LEU:CB    | 2.47                     | 0.45              |
| 6:XF:61:LEU:HD23  | 6:XF:63:TYR:OH    | 2.17                     | 0.45              |
| 11:XK:70:LYS:HA   | 11:XK:73:MET:HE3  | 1.98                     | 0.45              |
| 12:XL:113:ARG:NH2 | 12:XL:120:TYR:CE2 | 2.85                     | 0.45              |
| 13:XM:8:GLU:C     | 13:XM:9:ILE:CG2   | 2.90                     | 0.45              |
| 13:XM:15:VAL:O    | 13:XM:19:LEU:CD2  | 2.64                     | 0.45              |
| 16:XP:50:LYS:HD3  | 16:XP:50:LYS:C    | 2.41                     | 0.45              |
| 19:XS:69:HIS:O    | 19:XS:70:LYS:O    | 2.34                     | 0.45              |
| 20:XT:71:THR:HG22 | 20:XT:72:LEU:N    | 2.31                     | 0.45              |
| 25:YA:464:U:H2'   | 25:YA:465:G:O4'   | 2.17                     | 0.45              |
| 25:YA:819:A:C4    | 25:YA:1189:A:C2   | 3.04                     | 0.45              |
| 25:YA:1858:G:C6   | 25:YA:1883:G:C6   | 3.04                     | 0.45              |
| 26:YB:48:A:H4'    | 38:YS:95:HIS:CD2  | 2.51                     | 0.45              |
| 27:YD:198:ASN:ND2 | 27:YD:198:ASN:O   | 2.50                     | 0.45              |
| 28:YE:47:VAL:O    | 28:YE:47:VAL:HG23 | 2.16                     | 0.45              |
| 28:YE:95:ILE:HG22 | 28:YE:95:ILE:O    | 2.16                     | 0.45              |
| 33:YN:20:GLY:HA2  | 33:YN:61:ARG:HD2  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:52:VAL:O    | 36:YQ:53:ALA:C    | 2.59                     | 0.45              |
| 37:YR:29:LEU:N    | 37:YR:29:LEU:CD1  | 2.79                     | 0.45              |
| 37:YR:31:HIS:C    | 37:YR:33:ARG:H    | 2.25                     | 0.45              |
| 40:YU:95:LEU:HD13 | 41:YV:4:ILE:HD12  | 1.99                     | 0.45              |
| 42:YW:88:ARG:CB   | 42:YW:92:ARG:HB3  | 2.47                     | 0.45              |
| 44:YY:97:ARG:HG2  | 44:YY:97:ARG:HH11 | 1.82                     | 0.45              |
| 48:Y2:28:LYS:HB3  | 48:Y2:57:ILE:HG12 | 1.98                     | 0.45              |
| 1:QA:414:A:OP2    | 1:QA:428:G:N2     | 2.34                     | 0.45              |
| 1:QA:1074:G:C4'   | 2:QB:104:ASN:HB2  | 2.46                     | 0.45              |
| 1:QA:1095:U:H2'   | 1:QA:1096:C:C6    | 2.52                     | 0.45              |
| 3:QC:78:GLY:HA3   | 3:QC:83:ARG:HB3   | 1.98                     | 0.45              |
| 4:QD:11:LEU:O     | 4:QD:12:CYS:C     | 2.59                     | 0.45              |
| 4:QD:96:LEU:C     | 4:QD:98:GLU:N     | 2.72                     | 0.45              |
| 6:QF:35:ALA:HA    | 6:QF:67:MET:HB3   | 1.99                     | 0.45              |
| 9:QI:43:ALA:C     | 9:QI:45:ALA:N     | 2.73                     | 0.45              |
| 10:QJ:21:GLN:HG2  | 10:QJ:21:GLN:O    | 2.16                     | 0.45              |
| 13:QM:4:ILE:O     | 13:QM:5:ALA:C     | 2.60                     | 0.45              |
| 13:QM:28:ALA:C    | 13:QM:30:ALA:H    | 2.24                     | 0.45              |
| 20:QT:48:LYS:O    | 20:QT:49:ALA:C    | 2.59                     | 0.45              |
| 25:RA:1179:C:H2'  | 25:RA:1180:C:O4'  | 2.17                     | 0.45              |
| 25:RA:1257:C:H5'  | 29:RF:75:HIS:CE1  | 2.52                     | 0.45              |
| 25:RA:1266:G:O2'  | 25:RA:2012:G:O6   | 2.26                     | 0.45              |
| 25:RA:1309:G:OP1  | 53:R7:9:ARG:HD3   | 2.16                     | 0.45              |
| 25:RA:2174:C:H2'  | 25:RA:2175:C:C6   | 2.52                     | 0.45              |
| 25:RA:2286:A:H2'  | 52:R6:31:PRO:HG2  | 1.97                     | 0.45              |
| 25:RA:2591:C:OP2  | 27:RD:238:GLY:HA3 | 2.17                     | 0.45              |
| 27:RD:14:ARG:HG3  | 27:RD:15:PHE:N    | 2.31                     | 0.45              |
| 27:RD:36:PRO:HB3  | 27:RD:62:TYR:O    | 2.16                     | 0.45              |
| 27:RD:118:VAL:O   | 27:RD:129:ASN:HA  | 2.16                     | 0.45              |
| 27:RD:213:ARG:HA  | 27:RD:213:ARG:HD2 | 1.60                     | 0.45              |
| 28:RE:2:LYS:O     | 28:RE:199:ARG:HA  | 2.17                     | 0.45              |
| 29:RF:184:TYR:CE2 | 29:RF:188:ARG:HD2 | 2.52                     | 0.45              |
| 30:RG:36:LYS:O    | 30:RG:37:VAL:HG23 | 2.15                     | 0.45              |
| 30:RG:102:PHE:HA  | 30:RG:105:LYS:HE3 | 1.98                     | 0.45              |
| 35:RP:65:ARG:O    | 35:RP:66:GLY:C    | 2.60                     | 0.45              |
| 35:RP:144:GLU:OE1 | 35:RP:144:GLU:N   | 2.48                     | 0.45              |
| 36:RQ:11:LYS:HE2  | 36:RQ:87:LYS:HA   | 1.98                     | 0.45              |
| 41:RV:59:ALA:HB2  | 41:RV:96:ILE:HD13 | 1.97                     | 0.45              |
| 42:RW:14:PRO:O    | 42:RW:16:LYS:N    | 2.50                     | 0.45              |
| 42:RW:65:LEU:CD1  | 42:RW:68:ARG:NH1  | 2.75                     | 0.45              |
| 45:RZ:102:LEU:HB3 | 45:RZ:104:PHE:CE1 | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:R0:50:ASN:HB3  | 46:R0:63:VAL:HG22  | 1.99                     | 0.45              |
| 54:R8:16:ILE:CD1  | 54:R8:57:ARG:HG2   | 2.42                     | 0.45              |
| 1:XA:451:A:N7     | 1:XA:481:G:C2      | 2.85                     | 0.45              |
| 1:XA:939:G:H2'    | 1:XA:940:C:C6      | 2.52                     | 0.45              |
| 5:XE:48:ALA:C     | 5:XE:50:GLU:H      | 2.24                     | 0.45              |
| 6:XF:22:GLU:OE1   | 6:XF:82:ARG:NH2    | 2.46                     | 0.45              |
| 6:XF:68:PRO:HG3   | 6:XF:71:ARG:NH2    | 2.31                     | 0.45              |
| 6:XF:75:LEU:HD23  | 6:XF:75:LEU:C      | 2.41                     | 0.45              |
| 8:XH:97:VAL:CG1   | 8:XH:98:LYS:H      | 2.30                     | 0.45              |
| 8:XH:102:ARG:NH1  | 8:XH:105:ARG:CZ    | 2.80                     | 0.45              |
| 9:XI:71:SER:O     | 9:XI:72:GLY:C      | 2.58                     | 0.45              |
| 17:XQ:48:GLU:O    | 17:XQ:50:LYS:N     | 2.50                     | 0.45              |
| 19:XS:42:PRO:HD3  | 50:Y4:63:TYR:CE2   | 2.50                     | 0.45              |
| 25:YA:27:G:HO2'   | 25:YA:28:A:H8      | 1.63                     | 0.45              |
| 25:YA:278:A:H2'   | 25:YA:279:C:C6     | 2.52                     | 0.45              |
| 25:YA:1102:C:H2'  | 25:YA:1103:A:H5''  | 1.98                     | 0.45              |
| 25:YA:1264:G:H2'  | 25:YA:2014:A:N6    | 2.32                     | 0.45              |
| 25:YA:1543:A:HO2' | 25:YA:1544:C:H3'   | 1.80                     | 0.45              |
| 25:YA:1543:A:C2   | 25:YA:1545:A:C4    | 3.05                     | 0.45              |
| 26:YB:116:G:H4'   | 38:YS:54:LEU:HD13  | 1.98                     | 0.45              |
| 27:YD:25:THR:CG2  | 27:YD:25:THR:O     | 2.65                     | 0.45              |
| 27:YD:35:LYS:CE   | 27:YD:64:ILE:C     | 2.89                     | 0.45              |
| 27:YD:68:LYS:HD2  | 27:YD:70:TRP:CZ2   | 2.52                     | 0.45              |
| 27:YD:154:LYS:C   | 27:YD:155:LEU:HD12 | 2.41                     | 0.45              |
| 28:YE:154:LYS:C   | 28:YE:154:LYS:HD3  | 2.42                     | 0.45              |
| 29:YF:155:LEU:HA  | 29:YF:174:VAL:CG1  | 2.46                     | 0.45              |
| 29:YF:196:LEU:O   | 29:YF:200:GLU:HG2  | 2.17                     | 0.45              |
| 33:YN:10:GLU:HA   | 33:YN:11:PRO:HD3   | 1.74                     | 0.45              |
| 34:YO:22:ILE:HG12 | 34:YO:41:ALA:HA    | 1.98                     | 0.45              |
| 36:YQ:34:LEU:HB2  | 36:YQ:118:LEU:HD22 | 1.99                     | 0.45              |
| 40:YU:27:LEU:HD12 | 40:YU:31:SER:HB3   | 1.98                     | 0.45              |
| 40:YU:79:PHE:CE2  | 40:YU:83:LEU:HD13  | 2.51                     | 0.45              |
| 41:YV:95:LEU:C    | 41:YV:95:LEU:HD13  | 2.42                     | 0.45              |
| 42:YW:21:VAL:O    | 42:YW:21:VAL:HG12  | 2.17                     | 0.45              |
| 48:Y2:18:PRO:C    | 48:Y2:20:GLU:H     | 2.24                     | 0.45              |
| 52:Y6:15:GLU:OE2  | 52:Y6:44:ARG:NH1   | 2.49                     | 0.45              |
| 52:Y6:48:VAL:O    | 52:Y6:49:HIS:HB2   | 2.15                     | 0.45              |
| 54:Y8:52:LYS:O    | 54:Y8:52:LYS:CG    | 2.64                     | 0.45              |
| 1:QA:752:G:H1'    | 1:QA:754:C:N4      | 2.30                     | 0.45              |
| 1:QA:1446:A:N3    | 39:RT:118:ARG:HD2  | 2.32                     | 0.45              |
| 2:QB:170:GLU:C    | 2:QB:172:ILE:N     | 2.74                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:QB:240:GLN:HG2   | 2:QB:240:GLN:O    | 2.17                     | 0.45              |
| 4:QD:73:ARG:O      | 4:QD:74:GLN:C     | 2.58                     | 0.45              |
| 4:QD:199:ASN:O     | 4:QD:201:GLN:N    | 2.49                     | 0.45              |
| 5:QE:77:PRO:HG2    | 5:QE:142:LEU:HD22 | 1.98                     | 0.45              |
| 6:QF:9:VAL:HB      | 6:QF:87:ARG:HB2   | 1.97                     | 0.45              |
| 7:QG:95:ARG:HH11   | 7:QG:95:ARG:HG3   | 1.82                     | 0.45              |
| 10:QJ:38:ILE:CD1   | 10:QJ:71:LEU:HB3  | 2.46                     | 0.45              |
| 13:QM:57:ARG:HD2   | 13:QM:61:GLU:OE2  | 2.17                     | 0.45              |
| 13:QM:108:ARG:O    | 13:QM:111:LYS:N   | 2.48                     | 0.45              |
| 13:QM:110:ARG:HH11 | 13:QM:110:ARG:HG3 | 1.82                     | 0.45              |
| 15:QO:82:ILE:CG2   | 15:QO:83:GLU:N    | 2.79                     | 0.45              |
| 17:QQ:3:LYS:HD3    | 17:QQ:61:GLU:O    | 2.16                     | 0.45              |
| 20:QT:24:LEU:HD13  | 20:QT:24:LEU:O    | 2.16                     | 0.45              |
| 22:QV:53:G:HO2'    | 22:QV:54:U:H6     | 1.63                     | 0.45              |
| 25:RA:638:G:H2'    | 25:RA:639:U:O4'   | 2.16                     | 0.45              |
| 25:RA:678:C:H2'    | 25:RA:679:C:C6    | 2.52                     | 0.45              |
| 25:RA:2344:U:N3    | 52:R6:37:ARG:HD3  | 2.30                     | 0.45              |
| 27:RD:68:LYS:HD2   | 27:RD:70:TRP:CZ2  | 2.52                     | 0.45              |
| 27:RD:92:ILE:HD12  | 27:RD:104:TYR:HD2 | 1.81                     | 0.45              |
| 27:RD:109:ASP:HB2  | 27:RD:197:GLY:CA  | 2.46                     | 0.45              |
| 30:RG:78:SER:O     | 30:RG:79:ASN:C    | 2.59                     | 0.45              |
| 33:RN:46:VAL:HG13  | 33:RN:47:ALA:N    | 2.30                     | 0.45              |
| 33:RN:57:ALA:HA    | 33:RN:60:ILE:CD1  | 2.43                     | 0.45              |
| 35:RP:96:THR:HG22  | 35:RP:126:VAL:CB  | 2.47                     | 0.45              |
| 37:RR:84:ALA:O     | 37:RR:85:PRO:C    | 2.59                     | 0.45              |
| 38:RS:102:ALA:C    | 38:RS:104:GLY:N   | 2.73                     | 0.45              |
| 40:RU:15:LYS:O     | 40:RU:16:LYS:C    | 2.60                     | 0.45              |
| 40:RU:97:ASP:HA    | 40:RU:100:VAL:CG2 | 2.47                     | 0.45              |
| 44:RY:73:ARG:HE    | 44:RY:73:ARG:HB3  | 1.51                     | 0.45              |
| 44:RY:84:ARG:HD3   | 44:RY:86:ARG:HH11 | 1.82                     | 0.45              |
| 44:RY:87:LYS:C     | 44:RY:88:LYS:NZ   | 2.75                     | 0.45              |
| 52:R6:11:LEU:HD11  | 52:R6:51:GLU:HG3  | 1.98                     | 0.45              |
| 1:XA:560:U:O2'     | 1:XA:561:U:OP2    | 2.29                     | 0.45              |
| 1:XA:1443:G:H5'    | 1:XA:1446:A:OP2   | 2.17                     | 0.45              |
| 2:XB:22:LYS:O      | 2:XB:24:TRP:N     | 2.50                     | 0.45              |
| 2:XB:164:VAL:HB    | 2:XB:186:ALA:HB1  | 1.95                     | 0.45              |
| 3:XC:92:ALA:HB2    | 3:XC:99:VAL:HG11  | 1.99                     | 0.45              |
| 4:XD:101:LEU:HD21  | 4:XD:121:VAL:HG13 | 1.99                     | 0.45              |
| 5:XE:101:ILE:HD13  | 5:XE:101:ILE:H    | 1.82                     | 0.45              |
| 6:XF:29:ALA:O      | 6:XF:30:LEU:C     | 2.60                     | 0.45              |
| 7:XG:95:ARG:HH11   | 7:XG:95:ARG:HG3   | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:XI:47:LEU:HD22   | 9:XI:47:LEU:H      | 1.81                     | 0.45              |
| 10:XJ:63:PHE:HB3   | 14:XI:57:ARG:O     | 2.17                     | 0.45              |
| 12:XL:117:ARG:NH2  | 12:XL:124:LYS:HD3  | 2.32                     | 0.45              |
| 13:XM:28:ALA:C     | 13:XM:30:ALA:H     | 2.24                     | 0.45              |
| 13:XM:110:ARG:HH11 | 13:XM:110:ARG:HG3  | 1.82                     | 0.45              |
| 18:XR:44:LEU:C     | 18:XR:45:SER:O     | 2.59                     | 0.45              |
| 18:XR:63:GLN:HA    | 18:XR:63:GLN:OE1   | 2.17                     | 0.45              |
| 20:XT:36:LEU:C     | 20:XT:38:LYS:N     | 2.71                     | 0.45              |
| 25:YA:1799:G:H4'   | 25:YA:1800:C:O5'   | 2.17                     | 0.45              |
| 25:YA:2115:G:N2    | 25:YA:2165:G:O6    | 2.49                     | 0.45              |
| 25:YA:2212:A:H1'   | 25:YA:2215:G:C5    | 2.51                     | 0.45              |
| 25:YA:2712:U:OP1   | 25:YA:2714:G:H4'   | 2.16                     | 0.45              |
| 26:YB:44:G:H1'     | 26:YB:47:C:H42     | 1.82                     | 0.45              |
| 28:YE:21:VAL:HG23  | 28:YE:22:PRO:CD    | 2.46                     | 0.45              |
| 29:YF:61:GLY:O     | 29:YF:62:ARG:C     | 2.57                     | 0.45              |
| 34:YO:31:LYS:C     | 34:YO:32:TYR:CD2   | 2.95                     | 0.45              |
| 34:YO:53:LYS:N     | 34:YO:53:LYS:CD    | 2.69                     | 0.45              |
| 34:YO:104:ARG:NH2  | 39:YT:34:VAL:HG11  | 2.32                     | 0.45              |
| 36:YQ:5:ARG:O      | 36:YQ:6:ARG:O      | 2.35                     | 0.45              |
| 36:YQ:30:GLY:CA    | 36:YQ:107:ALA:HB2  | 2.39                     | 0.45              |
| 37:YR:12:ARG:HG3   | 37:YR:12:ARG:NH1   | 2.32                     | 0.45              |
| 44:YY:25:GLY:HA3   | 44:YY:39:VAL:CG1   | 2.47                     | 0.45              |
| 45:YZ:150:LEU:HB2  | 45:YZ:154:ASP:OD1  | 2.17                     | 0.45              |
| 1:QA:1446:A:C2     | 39:RT:118:ARG:HD2  | 2.52                     | 0.45              |
| 4:QD:94:LEU:O      | 4:QD:98:GLU:N      | 2.50                     | 0.45              |
| 5:QE:80:ILE:HG13   | 5:QE:82:VAL:HG23   | 1.99                     | 0.45              |
| 8:QH:86:ILE:CG1    | 8:QH:133:LEU:HD22  | 2.46                     | 0.45              |
| 10:QJ:29:ARG:HG2   | 10:QJ:29:ARG:HH11  | 1.81                     | 0.45              |
| 10:QJ:51:ARG:HG2   | 10:QJ:51:ARG:HH11  | 1.81                     | 0.45              |
| 11:QK:32:ILE:HD11  | 11:QK:72:ALA:HB2   | 1.96                     | 0.45              |
| 11:QK:83:ILE:HG12  | 11:QK:109:VAL:HG23 | 1.98                     | 0.45              |
| 13:QM:3:ARG:HD2    | 13:QM:9:ILE:CG1    | 2.45                     | 0.45              |
| 18:QR:63:GLN:HA    | 18:QR:63:GLN:OE1   | 2.17                     | 0.45              |
| 18:QR:82:THR:CG2   | 18:QR:83:GLU:N     | 2.79                     | 0.45              |
| 25:RA:1449:A:HO2'  | 25:RA:1530:G:N2    | 2.11                     | 0.45              |
| 25:RA:1678:G:N2    | 25:RA:1989:G:H22   | 2.13                     | 0.45              |
| 25:RA:1728:G:H3'   | 25:RA:1729:A:H5''  | 1.98                     | 0.45              |
| 25:RA:2635:C:H5''  | 28:RE:78:LEU:HA    | 1.98                     | 0.45              |
| 27:RD:44:ASN:HB2   | 27:RD:49:ILE:HA    | 1.93                     | 0.45              |
| 27:RD:79:VAL:HG21  | 27:RD:111:LEU:HD21 | 1.97                     | 0.45              |
| 27:RD:198:ASN:ND2  | 27:RD:198:ASN:O    | 2.50                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:RE:93:VAL:C     | 28:RE:95:ILE:N    | 2.75                     | 0.45              |
| 29:RF:123:LEU:HD12 | 29:RF:124:LEU:H   | 1.82                     | 0.45              |
| 29:RF:155:LEU:HA   | 29:RF:174:VAL:CG1 | 2.46                     | 0.45              |
| 33:RN:133:GLN:C    | 33:RN:134:ARG:HG2 | 2.41                     | 0.45              |
| 34:RO:107:ARG:O    | 34:RO:112:MET:HE1 | 2.17                     | 0.45              |
| 35:RP:115:LEU:CB   | 35:RP:131:SER:HB2 | 2.47                     | 0.45              |
| 37:RR:17:ARG:O     | 37:RR:20:LEU:HB3  | 2.17                     | 0.45              |
| 41:RV:5:VAL:HG13   | 41:RV:14:VAL:HG21 | 1.98                     | 0.45              |
| 41:RV:61:VAL:HA    | 41:RV:94:LEU:HD23 | 1.97                     | 0.45              |
| 41:RV:69:LYS:HG3   | 41:RV:87:HIS:O    | 2.17                     | 0.45              |
| 41:RV:95:LEU:HD13  | 41:RV:95:LEU:C    | 2.42                     | 0.45              |
| 47:R1:49:VAL:HG12  | 47:R1:51:VAL:HG23 | 1.99                     | 0.45              |
| 47:R1:80:LEU:CB    | 47:R1:81:LYS:HE2  | 2.44                     | 0.45              |
| 1:XA:474:G:H2'     | 1:XA:475:G:H8     | 1.81                     | 0.45              |
| 1:XA:603:U:H2'     | 1:XA:604:G:H8     | 1.82                     | 0.45              |
| 1:XA:981:U:H2'     | 1:XA:982:U:C5     | 2.52                     | 0.45              |
| 1:XA:1314:C:C5     | 19:XS:4:SER:HB2   | 2.51                     | 0.45              |
| 3:XC:172:ARG:C     | 3:XC:173:VAL:HG23 | 2.42                     | 0.45              |
| 5:XE:12:LEU:HD21   | 5:XE:14:ARG:HB3   | 1.98                     | 0.45              |
| 6:XF:101:ALA:HA    | 18:XR:28:GLU:CG   | 2.46                     | 0.45              |
| 7:XG:16:LEU:HD13   | 9:XI:45:ALA:HB2   | 1.99                     | 0.45              |
| 7:XG:111:ARG:HD2   | 7:XG:123:GLU:HB2  | 1.99                     | 0.45              |
| 8:XH:122:ARG:O     | 8:XH:123:GLU:C    | 2.60                     | 0.45              |
| 10:XJ:6:ILE:O      | 10:XJ:71:LEU:HD12 | 2.17                     | 0.45              |
| 10:XJ:22:LYS:C     | 10:XJ:22:LYS:CD   | 2.90                     | 0.45              |
| 11:XK:124:LYS:O    | 11:XK:126:ARG:N   | 2.40                     | 0.45              |
| 13:XM:56:LEU:HD13  | 13:XM:56:LEU:O    | 2.17                     | 0.45              |
| 15:XO:25:THR:HG22  | 15:XO:70:LEU:HD22 | 1.99                     | 0.45              |
| 15:XO:74:ASP:C     | 15:XO:76:GLU:H    | 2.24                     | 0.45              |
| 15:XO:82:ILE:CG2   | 15:XO:83:GLU:N    | 2.79                     | 0.45              |
| 17:XQ:82:MET:C     | 17:XQ:84:LEU:H    | 2.25                     | 0.45              |
| 25:YA:299:A:N1     | 25:YA:322:A:O2'   | 2.43                     | 0.45              |
| 25:YA:612:G:N2     | 25:YA:617:G:C5    | 2.85                     | 0.45              |
| 25:YA:629:G:H5'    | 25:YA:650:C:O2'   | 2.16                     | 0.45              |
| 25:YA:747:U:C2     | 51:Y5:2:ALA:HB3   | 2.52                     | 0.45              |
| 25:YA:1291:C:H2'   | 25:YA:1292:U:C6   | 2.52                     | 0.45              |
| 25:YA:1441:G:H2'   | 25:YA:1442:G:H8   | 1.82                     | 0.45              |
| 25:YA:1872:A:H5'   | 25:YA:1878:G:OP2  | 2.17                     | 0.45              |
| 25:YA:1952:A:C5    | 34:YO:22:ILE:HD12 | 2.52                     | 0.45              |
| 25:YA:2316:C:H2'   | 25:YA:2317:C:C6   | 2.51                     | 0.45              |
| 25:YA:2619:C:H1'   | 28:YE:156:MET:HE1 | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2656:U:H3    | 25:YA:2665:A:H2    | 1.65                     | 0.45              |
| 25:YA:2689:U:H4'   | 25:YA:2690:C:O5'   | 2.16                     | 0.45              |
| 26:YB:15:A:H4'     | 26:YB:15:A:OP1     | 2.16                     | 0.45              |
| 28:YE:2:LYS:O      | 28:YE:199:ARG:HA   | 2.17                     | 0.45              |
| 28:YE:4:ILE:HG12   | 28:YE:91:VAL:HG11  | 1.99                     | 0.45              |
| 28:YE:199:ARG:HH11 | 28:YE:199:ARG:HG3  | 1.82                     | 0.45              |
| 29:YF:198:ALA:C    | 29:YF:200:GLU:H    | 2.25                     | 0.45              |
| 33:YN:5:VAL:O      | 33:YN:5:VAL:HG13   | 2.16                     | 0.45              |
| 33:YN:22:THR:O     | 33:YN:60:ILE:HG22  | 2.16                     | 0.45              |
| 34:YO:19:ILE:HD13  | 34:YO:19:ILE:H     | 1.82                     | 0.45              |
| 34:YO:97:ARG:H     | 34:YO:117:LEU:CD2  | 2.24                     | 0.45              |
| 34:YO:107:ARG:O    | 34:YO:112:MET:HE1  | 2.17                     | 0.45              |
| 35:YP:75:ILE:HG12  | 35:YP:77:ARG:NH1   | 2.32                     | 0.45              |
| 35:YP:75:ILE:HG12  | 35:YP:77:ARG:HH12  | 1.82                     | 0.45              |
| 35:YP:92:GLU:HA    | 35:YP:123:LEU:HD23 | 1.99                     | 0.45              |
| 36:YQ:58:PHE:O     | 36:YQ:58:PHE:CD1   | 2.70                     | 0.45              |
| 36:YQ:65:PHE:O     | 36:YQ:66:ILE:CG1   | 2.48                     | 0.45              |
| 36:YQ:133:ARG:CG   | 36:YQ:134:ARG:N    | 2.78                     | 0.45              |
| 37:YR:17:ARG:O     | 37:YR:20:LEU:HB3   | 2.16                     | 0.45              |
| 38:YS:83:LYS:CE    | 38:YS:109:GLY:HA2  | 2.47                     | 0.45              |
| 39:YT:23:ARG:CB    | 39:YT:24:PRO:HD2   | 2.40                     | 0.45              |
| 41:YV:61:VAL:O     | 41:YV:61:VAL:HG22  | 2.16                     | 0.45              |
| 41:YV:69:LYS:HG3   | 41:YV:87:HIS:O     | 2.17                     | 0.45              |
| 42:YW:14:PRO:O     | 42:YW:16:LYS:N     | 2.50                     | 0.45              |
| 50:Y4:51:ASP:O     | 50:Y4:51:ASP:CG    | 2.60                     | 0.45              |
| 50:Y4:68:ARG:O     | 50:Y4:69:LYS:HB2   | 2.17                     | 0.45              |
| 52:Y6:18:ARG:O     | 52:Y6:19:ARG:O     | 2.33                     | 0.45              |
| 53:Y7:2:LYS:HG2    | 53:Y7:3:ARG:N      | 2.31                     | 0.45              |
| 1:QA:359:U:H2'     | 1:QA:360:A:C8      | 2.52                     | 0.45              |
| 1:QA:636:U:H2'     | 1:QA:637:G:C8      | 2.52                     | 0.45              |
| 1:QA:688:G:H2'     | 1:QA:689:C:H6      | 1.81                     | 0.45              |
| 2:QB:75:LYS:C      | 2:QB:77:ALA:H      | 2.24                     | 0.45              |
| 2:QB:214:ILE:HD13  | 2:QB:217:ARG:HH22  | 1.81                     | 0.45              |
| 3:QC:43:LEU:HD11   | 3:QC:66:VAL:HG11   | 1.98                     | 0.45              |
| 3:QC:172:ARG:C     | 3:QC:173:VAL:HG23  | 2.42                     | 0.45              |
| 4:QD:120:LEU:CD2   | 4:QD:125:HIS:HB2   | 2.46                     | 0.45              |
| 5:QE:7:GLU:HB3     | 5:QE:112:LEU:HD13  | 1.99                     | 0.45              |
| 9:QI:71:SER:C      | 9:QI:73:GLN:N      | 2.74                     | 0.45              |
| 10:QJ:22:LYS:C     | 10:QJ:22:LYS:CD    | 2.90                     | 0.45              |
| 10:QJ:33:GLN:HB2   | 10:QJ:75:ILE:HD11  | 1.99                     | 0.45              |
| 10:QJ:63:PHE:HB3   | 14:QN:57:ARG:O     | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:QM:15:VAL:O     | 13:QM:19:LEU:CD2  | 2.64                     | 0.45              |
| 13:QM:39:ILE:HD12  | 13:QM:56:LEU:HD23 | 1.99                     | 0.45              |
| 16:QP:39:TYR:CZ    | 16:QP:41:PRO:HB3  | 2.52                     | 0.45              |
| 19:QS:13:ASP:O     | 19:QS:14:HIS:C    | 2.60                     | 0.45              |
| 19:QS:69:HIS:O     | 19:QS:70:LYS:O    | 2.34                     | 0.45              |
| 25:RA:38:A:N3      | 29:RF:48:THR:OG1  | 2.48                     | 0.45              |
| 25:RA:1819:A:H4'   | 25:RA:1820:U:O5'  | 2.16                     | 0.45              |
| 25:RA:1993:U:H4'   | 28:RE:128:SER:OG  | 2.17                     | 0.45              |
| 25:RA:2477:C:H2'   | 55:R9:1:MET:HG3   | 1.98                     | 0.45              |
| 28:RE:2:LYS:HG2    | 28:RE:95:ILE:HG22 | 1.99                     | 0.45              |
| 28:RE:36:ARG:HH11  | 28:RE:36:ARG:CB   | 2.28                     | 0.45              |
| 28:RE:77:ILE:O     | 28:RE:78:LEU:O    | 2.35                     | 0.45              |
| 29:RF:119:ARG:HH11 | 29:RF:119:ARG:CG  | 2.29                     | 0.45              |
| 29:RF:196:LEU:O    | 29:RF:200:GLU:HG2 | 2.17                     | 0.45              |
| 30:RG:110:ALA:C    | 30:RG:112:PRO:HD2 | 2.42                     | 0.45              |
| 30:RG:129:GLY:O    | 30:RG:130:ASN:OD1 | 2.34                     | 0.45              |
| 32:RI:2:LYS:HA     | 32:RI:20:ASP:HA   | 1.99                     | 0.45              |
| 32:RI:4:ILE:HG22   | 32:RI:16:GLY:HA2  | 1.98                     | 0.45              |
| 34:RO:2:ILE:HD11   | 34:RO:82:ASN:ND2  | 2.16                     | 0.45              |
| 35:RP:115:LEU:HA   | 35:RP:134:ALA:CB  | 2.47                     | 0.45              |
| 39:RT:118:ARG:O    | 39:RT:119:LYS:C   | 2.60                     | 0.45              |
| 41:RV:4:ILE:HG22   | 41:RV:39:LEU:HD23 | 1.98                     | 0.45              |
| 41:RV:5:VAL:HG22   | 41:RV:14:VAL:CG2  | 2.46                     | 0.45              |
| 42:RW:67:ASP:OD2   | 42:RW:67:ASP:N    | 2.50                     | 0.45              |
| 43:RX:35:THR:O     | 43:RX:35:THR:HG23 | 2.16                     | 0.45              |
| 47:R1:48:LYS:HA    | 47:R1:60:PHE:O    | 2.17                     | 0.45              |
| 47:R1:60:PHE:HZ    | 47:R1:90:ILE:HG21 | 1.82                     | 0.45              |
| 54:R8:9:GLY:O      | 54:R8:13:ARG:HG2  | 2.16                     | 0.45              |
| 54:R8:36:LYS:HB3   | 54:R8:40:GLU:HG2  | 1.99                     | 0.45              |
| 1:XA:401:C:O2'     | 1:XA:621:A:N3     | 2.49                     | 0.45              |
| 1:XA:925:G:N2      | 1:XA:1503:A:OP1   | 2.49                     | 0.45              |
| 1:XA:1313:U:OP1    | 19:XS:5:LEU:HB2   | 2.17                     | 0.45              |
| 5:XE:10:MET:HB2    | 5:XE:32:VAL:HG22  | 1.93                     | 0.45              |
| 5:XE:52:PRO:HB2    | 5:XE:53:LEU:HD12  | 1.97                     | 0.45              |
| 5:XE:147:ASP:N     | 5:XE:147:ASP:OD2  | 2.50                     | 0.45              |
| 7:XG:45:ASP:O      | 7:XG:49:ILE:HG12  | 2.17                     | 0.45              |
| 10:XJ:51:ARG:HH11  | 10:XJ:51:ARG:HG2  | 1.81                     | 0.45              |
| 10:XJ:54:PHE:CE2   | 10:XJ:55:LYS:HD2  | 2.52                     | 0.45              |
| 11:XK:75:TYR:N     | 11:XK:75:TYR:CD1  | 2.85                     | 0.45              |
| 12:XL:120:TYR:N    | 12:XL:120:TYR:CD1 | 2.85                     | 0.45              |
| 13:XM:77:ASN:ND2   | 50:Y4:71:ARG:NH1  | 2.65                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:XP:22:THR:CA    | 16:XP:33:ILE:HG12  | 2.42                     | 0.45              |
| 16:XP:47:ASP:C     | 16:XP:49:LEU:N     | 2.75                     | 0.45              |
| 16:XP:58:TYR:C     | 16:XP:58:TYR:CD1   | 2.94                     | 0.45              |
| 17:XQ:59:ILE:N     | 17:XQ:59:ILE:CD1   | 2.78                     | 0.45              |
| 19:XS:45:VAL:O     | 19:XS:62:ILE:O     | 2.35                     | 0.45              |
| 20:XT:44:ALA:O     | 20:XT:91:LEU:HB3   | 2.16                     | 0.45              |
| 25:YA:49:A:N7      | 25:YA:120:U:C5     | 2.85                     | 0.45              |
| 25:YA:270(R):G:H1' | 47:Y1:78:LYS:HZ1   | 1.82                     | 0.45              |
| 25:YA:994:C:O2     | 41:YV:10:LYS:HE2   | 2.17                     | 0.45              |
| 25:YA:2020:A:H5'   | 51:Y5:12:SER:HB3   | 1.99                     | 0.45              |
| 25:YA:2052:G:H2'   | 25:YA:2053:G:H8    | 1.81                     | 0.45              |
| 25:YA:2250:G:C4    | 36:YQ:82:ARG:HG3   | 2.52                     | 0.45              |
| 25:YA:2285:C:H5    | 52:Y6:27:LYS:HE2   | 1.82                     | 0.45              |
| 27:YD:226:MET:H    | 27:YD:226:MET:HG2  | 1.53                     | 0.45              |
| 33:YN:7:LYS:HD3    | 33:YN:9:VAL:H      | 1.81                     | 0.45              |
| 33:YN:65:LYS:O     | 33:YN:66:LYS:C     | 2.60                     | 0.45              |
| 35:YP:45:LEU:CD1   | 35:YP:45:LEU:N     | 2.79                     | 0.45              |
| 35:YP:112:LEU:CD1  | 35:YP:114:ILE:HG23 | 2.47                     | 0.45              |
| 36:YQ:93:TYR:N     | 36:YQ:93:TYR:CD1   | 2.85                     | 0.45              |
| 44:YY:57:GLN:O     | 44:YY:58:GLY:C     | 2.60                     | 0.45              |
| 44:YY:87:LYS:C     | 44:YY:88:LYS:NZ    | 2.75                     | 0.45              |
| 52:Y6:7:ILE:O      | 52:Y6:8:LYS:HG2    | 2.17                     | 0.45              |
| 52:Y6:7:ILE:HG23   | 52:Y6:8:LYS:N      | 2.32                     | 0.45              |
| 54:Y8:36:LYS:HB3   | 54:Y8:40:GLU:HG2   | 1.99                     | 0.45              |
| 1:QA:643:C:H2'     | 1:QA:644:G:C8      | 2.52                     | 0.44              |
| 1:QA:1366:C:H2'    | 1:QA:1367:C:C6     | 2.51                     | 0.44              |
| 2:QB:109:SER:C     | 2:QB:111:ARG:N     | 2.73                     | 0.44              |
| 4:QD:178:VAL:O     | 4:QD:181:MET:N     | 2.50                     | 0.44              |
| 5:QE:12:LEU:HB3    | 5:QE:31:LEU:CB     | 2.46                     | 0.44              |
| 6:QF:29:ALA:O      | 6:QF:30:LEU:C      | 2.60                     | 0.44              |
| 7:QG:26:PHE:HZ     | 7:QG:120:ILE:HG23  | 1.83                     | 0.44              |
| 9:QI:20:ARG:O      | 9:QI:21:PRO:C      | 2.59                     | 0.44              |
| 10:QJ:62:HIS:N     | 10:QJ:62:HIS:CD2   | 2.85                     | 0.44              |
| 16:QP:58:TYR:CD1   | 16:QP:58:TYR:C     | 2.94                     | 0.44              |
| 19:QS:15:LEU:O     | 19:QS:16:LEU:C     | 2.60                     | 0.44              |
| 19:QS:41:VAL:HG13  | 19:QS:44:MET:CB    | 2.38                     | 0.44              |
| 20:QT:28:ALA:O     | 20:QT:30:LYS:N     | 2.50                     | 0.44              |
| 25:RA:29:U:H2'     | 25:RA:30:G:C8      | 2.52                     | 0.44              |
| 25:RA:537:C:O2     | 33:RN:45:ASN:ND2   | 2.50                     | 0.44              |
| 25:RA:558:G:P      | 33:RN:111:PRO:HD2  | 2.56                     | 0.44              |
| 25:RA:1853:A:H2'   | 25:RA:1854:A:C8    | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2590:A:H2'   | 25:RA:2591:C:C6    | 2.52                     | 0.44              |
| 26:RB:16:G:H2'     | 26:RB:17:C:H6      | 1.81                     | 0.44              |
| 26:RB:79:C:H2'     | 26:RB:80:U:O4'     | 2.17                     | 0.44              |
| 27:RD:48:ARG:HG3   | 27:RD:48:ARG:NH1   | 2.31                     | 0.44              |
| 27:RD:145:VAL:HG12 | 27:RD:146:GLU:N    | 2.32                     | 0.44              |
| 27:RD:166:GLN:HA   | 27:RD:166:GLN:NE2  | 2.32                     | 0.44              |
| 27:RD:176:ARG:HH11 | 27:RD:176:ARG:CG   | 2.30                     | 0.44              |
| 28:RE:154:LYS:HD3  | 28:RE:154:LYS:C    | 2.42                     | 0.44              |
| 30:RG:16:ARG:CZ    | 30:RG:31:VAL:HG11  | 2.47                     | 0.44              |
| 30:RG:44:GLY:HA2   | 30:RG:88:ILE:HD11  | 1.99                     | 0.44              |
| 30:RG:67:LYS:CE    | 50:R4:6:HIS:NE2    | 2.74                     | 0.44              |
| 31:RH:53:GLU:OE1   | 31:RH:53:GLU:HA    | 2.16                     | 0.44              |
| 34:RO:19:ILE:HD13  | 34:RO:19:ILE:H     | 1.82                     | 0.44              |
| 34:RO:78:ARG:HH21  | 39:RT:103:ARG:HH22 | 1.64                     | 0.44              |
| 36:RQ:10:ARG:O     | 36:RQ:11:LYS:CB    | 2.64                     | 0.44              |
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:CG   | 2.25                     | 0.44              |
| 40:RU:86:ALA:CB    | 40:RU:88:ILE:HD11  | 2.48                     | 0.44              |
| 42:RW:21:VAL:O     | 42:RW:21:VAL:HG12  | 2.17                     | 0.44              |
| 45:RZ:60:GLU:HA    | 45:RZ:66:SER:HA    | 1.99                     | 0.44              |
| 46:R0:11:ARG:H     | 46:R0:11:ARG:HG3   | 1.53                     | 0.44              |
| 48:R2:18:PRO:C     | 48:R2:20:GLU:H     | 2.24                     | 0.44              |
| 52:R6:9:LEU:CD1    | 52:R6:26:ASN:ND2   | 2.80                     | 0.44              |
| 53:R7:24:THR:O     | 53:R7:28:ARG:HG3   | 2.16                     | 0.44              |
| 1:XA:603:U:H2'     | 1:XA:604:G:C8      | 2.52                     | 0.44              |
| 1:XA:612:C:O2      | 1:XA:629:G:N2      | 2.51                     | 0.44              |
| 1:XA:778:G:O2'     | 11:XK:119:CYS:HB3  | 2.18                     | 0.44              |
| 1:XA:923:A:N6      | 1:XA:1392:G:O6     | 2.49                     | 0.44              |
| 1:XA:1349:A:P      | 9:XI:118:LYS:NZ    | 2.91                     | 0.44              |
| 1:XA:1510:U:H2'    | 1:XA:1511:G:C8     | 2.52                     | 0.44              |
| 2:XB:30:ARG:O      | 2:XB:31:TYR:HD2    | 2.00                     | 0.44              |
| 2:XB:68:ILE:HB     | 2:XB:70:PHE:HE1    | 1.82                     | 0.44              |
| 2:XB:98:LEU:O      | 2:XB:101:MET:HG3   | 2.17                     | 0.44              |
| 2:XB:188:ALA:CB    | 2:XB:200:ILE:HG23  | 2.47                     | 0.44              |
| 2:XB:229:VAL:HG12  | 2:XB:229:VAL:O     | 2.17                     | 0.44              |
| 5:XE:78:HIS:CG     | 8:XH:104:ARG:HG2   | 2.52                     | 0.44              |
| 5:XE:150:ARG:HG2   | 5:XE:150:ARG:O     | 2.16                     | 0.44              |
| 7:XG:26:PHE:HZ     | 7:XG:120:ILE:HG23  | 1.82                     | 0.44              |
| 9:XI:5:TYR:CD2     | 9:XI:6:GLY:N       | 2.85                     | 0.44              |
| 10:XJ:54:PHE:CD2   | 10:XJ:55:LYS:HD2   | 2.52                     | 0.44              |
| 13:XM:108:ARG:O    | 13:XM:111:LYS:N    | 2.48                     | 0.44              |
| 25:YA:246:C:N4     | 54:Y8:8:LYS:HG3    | 2.31                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:262:A:H2'   | 25:YA:263:C:O4'    | 2.16                     | 0.44              |
| 25:YA:1032:A:H2   | 25:YA:1122:G:H22   | 1.63                     | 0.44              |
| 25:YA:2168:G:H8   | 25:YA:2168:G:OP2   | 2.00                     | 0.44              |
| 25:YA:2477:C:H2'  | 55:Y9:1:MET:CG     | 2.47                     | 0.44              |
| 27:YD:52:ARG:HB2  | 27:YD:53:PHE:CD2   | 2.52                     | 0.44              |
| 29:YF:144:LYS:C   | 29:YF:146:ALA:N    | 2.75                     | 0.44              |
| 32:YI:135:GLU:HB2 | 32:YI:136:VAL:H    | 1.64                     | 0.44              |
| 33:YN:99:LEU:O    | 33:YN:100:GLU:C    | 2.60                     | 0.44              |
| 34:YO:97:ARG:HA   | 34:YO:117:LEU:HD22 | 1.99                     | 0.44              |
| 34:YO:112:MET:O   | 34:YO:113:LYS:C    | 2.60                     | 0.44              |
| 35:YP:65:ARG:O    | 35:YP:66:GLY:C     | 2.59                     | 0.44              |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:CA   | 2.47                     | 0.44              |
| 39:YT:36:GLU:CG   | 39:YT:41:ARG:HD3   | 2.46                     | 0.44              |
| 40:YU:15:LYS:O    | 40:YU:16:LYS:C     | 2.60                     | 0.44              |
| 41:YV:67:GLY:O    | 41:YV:68:LYS:C     | 2.59                     | 0.44              |
| 47:Y1:10:LYS:HD2  | 47:Y1:66:HIS:HE1   | 1.82                     | 0.44              |
| 1:QA:439:A:OP2    | 1:QA:493:G:N1      | 2.51                     | 0.44              |
| 1:QA:598:U:H4'    | 8:QH:94:TYR:CD2    | 2.52                     | 0.44              |
| 1:QA:1346:A:C4    | 7:QG:10:ARG:NH1    | 2.85                     | 0.44              |
| 2:QB:95:GLN:NE2   | 2:QB:96:ARG:NH1    | 2.65                     | 0.44              |
| 2:QB:189:ASP:OD2  | 2:QB:205:ASP:OD1   | 2.35                     | 0.44              |
| 2:QB:221:LEU:HD13 | 2:QB:221:LEU:C     | 2.42                     | 0.44              |
| 4:QD:25:ARG:CZ    | 4:QD:30:LYS:HE3    | 2.46                     | 0.44              |
| 5:QE:31:LEU:HD23  | 5:QE:45:PHE:CD1    | 2.53                     | 0.44              |
| 7:QG:111:ARG:HD2  | 7:QG:123:GLU:HB2   | 1.99                     | 0.44              |
| 8:QH:64:LYS:HB3   | 8:QH:79:VAL:HG21   | 1.98                     | 0.44              |
| 13:QM:56:LEU:HD13 | 13:QM:56:LEU:O     | 2.17                     | 0.44              |
| 15:QO:29:VAL:HB   | 15:QO:81:LEU:HD21  | 1.99                     | 0.44              |
| 20:QT:44:ALA:HB1  | 20:QT:91:LEU:HB2   | 2.00                     | 0.44              |
| 20:QT:89:ARG:HH12 | 20:QT:106:ALA:HB1  | 1.82                     | 0.44              |
| 25:RA:662:G:H5'   | 35:RP:15:ARG:HA    | 1.97                     | 0.44              |
| 25:RA:971:C:H2'   | 25:RA:972:G:O4'    | 2.17                     | 0.44              |
| 25:RA:2377:A:H2   | 38:RS:18:ILE:HD11  | 1.83                     | 0.44              |
| 29:RF:7:TYR:N     | 29:RF:7:TYR:CD1    | 2.85                     | 0.44              |
| 30:RG:6:ALA:HB3   | 30:RG:104:GLU:OE2  | 2.16                     | 0.44              |
| 31:RH:149:ARG:HA  | 31:RH:162:ILE:HG21 | 1.99                     | 0.44              |
| 34:RO:22:ILE:HG12 | 34:RO:41:ALA:HA    | 1.98                     | 0.44              |
| 42:RW:74:ALA:O    | 42:RW:75:TYR:CB    | 2.65                     | 0.44              |
| 49:R3:39:ASP:O    | 49:R3:40:THR:C     | 2.59                     | 0.44              |
| 50:R4:51:ASP:O    | 50:R4:51:ASP:CG    | 2.60                     | 0.44              |
| 51:R5:56:LYS:O    | 51:R5:58:LEU:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:R8:17:THR:O    | 54:R8:20:GLY:N    | 2.46                     | 0.44              |
| 54:R8:47:LYS:HD2  | 54:R8:48:PHE:N    | 2.33                     | 0.44              |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:C8  | 2.52                     | 0.44              |
| 1:XA:452:A:H4'    | 16:XP:72:ARG:NH2  | 2.31                     | 0.44              |
| 1:XA:1122:U:O4    | 1:XA:1123:A:N6    | 2.50                     | 0.44              |
| 1:XA:1182:G:H4'   | 1:XA:1183:A:H5''  | 1.98                     | 0.44              |
| 1:XA:1364:U:O2'   | 1:XA:1365:G:OP1   | 2.35                     | 0.44              |
| 2:XB:128:GLU:O    | 2:XB:129:GLU:C    | 2.61                     | 0.44              |
| 2:XB:170:GLU:C    | 2:XB:172:ILE:N    | 2.74                     | 0.44              |
| 4:XD:206:PHE:CD2  | 4:XD:207:TYR:CE1  | 3.05                     | 0.44              |
| 5:XE:82:VAL:HG12  | 5:XE:83:GLU:H     | 1.77                     | 0.44              |
| 6:XF:23:LYS:HG2   | 6:XF:27:GLN:OE1   | 2.18                     | 0.44              |
| 9:XI:7:THR:O      | 9:XI:83:ARG:CD    | 2.66                     | 0.44              |
| 13:XM:53:VAL:HG12 | 13:XM:57:ARG:HH12 | 1.82                     | 0.44              |
| 19:XS:13:ASP:O    | 19:XS:14:HIS:C    | 2.60                     | 0.44              |
| 19:XS:15:LEU:O    | 19:XS:16:LEU:C    | 2.60                     | 0.44              |
| 20:XT:56:MET:HG3  | 20:XT:88:VAL:HG21 | 1.98                     | 0.44              |
| 25:YA:80:G:N2     | 25:YA:106:C:O2    | 2.46                     | 0.44              |
| 25:YA:704:G:H1'   | 25:YA:727:A:N6    | 2.33                     | 0.44              |
| 25:YA:1014:U:H2'  | 25:YA:1015:G:H8   | 1.82                     | 0.44              |
| 25:YA:1791:A:H3'  | 25:YA:1792:G:H8   | 1.82                     | 0.44              |
| 25:YA:1820:U:H4'  | 25:YA:1821:A:OP2  | 2.16                     | 0.44              |
| 27:YD:177:LEU:O   | 27:YD:179:SER:N   | 2.51                     | 0.44              |
| 27:YD:214:TRP:C   | 27:YD:216:GLY:H   | 2.26                     | 0.44              |
| 30:YG:129:GLY:HA2 | 30:YG:169:ALA:HB2 | 1.99                     | 0.44              |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:HE3 | 1.98                     | 0.44              |
| 32:YI:128:LEU:O   | 32:YI:138:ILE:N   | 2.36                     | 0.44              |
| 33:YN:112:LEU:O   | 33:YN:116:LEU:HG  | 2.16                     | 0.44              |
| 35:YP:21:ARG:HA   | 35:YP:21:ARG:HE   | 1.82                     | 0.44              |
| 36:YQ:66:ILE:O    | 36:YQ:104:PHE:N   | 2.49                     | 0.44              |
| 38:YS:3:ARG:O     | 38:YS:4:LEU:O     | 2.35                     | 0.44              |
| 39:YT:24:PRO:HD3  | 39:YT:52:ILE:HD12 | 1.99                     | 0.44              |
| 40:YU:91:ASP:C    | 40:YU:93:LYS:N    | 2.74                     | 0.44              |
| 42:YW:31:GLU:O    | 42:YW:32:ALA:C    | 2.60                     | 0.44              |
| 47:Y1:48:LYS:HA   | 47:Y1:60:PHE:O    | 2.17                     | 0.44              |
| 51:Y5:56:LYS:O    | 51:Y5:58:LEU:N    | 2.50                     | 0.44              |
| 2:QB:98:LEU:O     | 2:QB:101:MET:HG3  | 2.17                     | 0.44              |
| 3:QC:6:HIS:C      | 3:QC:8:ILE:N      | 2.76                     | 0.44              |
| 3:QC:73:PRO:O     | 3:QC:77:ILE:HG13  | 2.16                     | 0.44              |
| 4:QD:49:ARG:O     | 4:QD:50:ARG:C     | 2.60                     | 0.44              |
| 4:QD:199:ASN:C    | 4:QD:201:GLN:H    | 2.25                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:QI:7:THR:O      | 9:QI:83:ARG:CD    | 2.66                     | 0.44              |
| 13:QM:16:ASP:O    | 13:QM:19:LEU:HD23 | 2.17                     | 0.44              |
| 17:QQ:13:ASP:O    | 17:QQ:15:MET:N    | 2.51                     | 0.44              |
| 17:QQ:48:GLU:O    | 17:QQ:50:LYS:N    | 2.50                     | 0.44              |
| 17:QQ:66:SER:O    | 17:QQ:67:LYS:C    | 2.61                     | 0.44              |
| 25:RA:222:A:HO2'  | 25:RA:223:A:P     | 2.41                     | 0.44              |
| 25:RA:298:G:H5''  | 25:RA:299:A:OP1   | 2.17                     | 0.44              |
| 25:RA:639:U:H2'   | 25:RA:640:C:C6    | 2.52                     | 0.44              |
| 25:RA:861:A:H2'   | 25:RA:862:G:O4'   | 2.18                     | 0.44              |
| 25:RA:1005:C:O2'  | 33:RN:28:THR:HG21 | 2.16                     | 0.44              |
| 25:RA:1058:G:N2   | 25:RA:1080:C:O2   | 2.42                     | 0.44              |
| 25:RA:1106:G:H2'  | 25:RA:1107:G:H8   | 1.83                     | 0.44              |
| 25:RA:2328:A:H2'  | 25:RA:2329:G:C8   | 2.52                     | 0.44              |
| 25:RA:2329:G:H2'  | 25:RA:2330:G:C8   | 2.51                     | 0.44              |
| 25:RA:2723:C:OP1  | 37:RR:3:HIS:HD2   | 2.00                     | 0.44              |
| 27:RD:143:HIS:HD2 | 27:RD:144:ALA:HB2 | 1.83                     | 0.44              |
| 28:RE:36:ARG:O    | 28:RE:37:ARG:C    | 2.59                     | 0.44              |
| 28:RE:101:ARG:HD2 | 28:RE:171:GLU:HA  | 1.98                     | 0.44              |
| 31:RH:51:ARG:HG3  | 31:RH:51:ARG:NH1  | 2.30                     | 0.44              |
| 33:RN:36:GLY:O    | 33:RN:42:TRP:CE3  | 2.69                     | 0.44              |
| 34:RO:104:ARG:NH2 | 39:RT:34:VAL:HG11 | 2.32                     | 0.44              |
| 35:RP:75:ILE:HG12 | 35:RP:77:ARG:HH12 | 1.82                     | 0.44              |
| 38:RS:3:ARG:O     | 38:RS:4:LEU:O     | 2.35                     | 0.44              |
| 38:RS:78:LEU:HD21 | 38:RS:108:GLY:CA  | 2.47                     | 0.44              |
| 39:RT:49:VAL:O    | 39:RT:49:VAL:CG1  | 2.64                     | 0.44              |
| 40:RU:66:ASN:CB   | 40:RU:76:TYR:HB2  | 2.44                     | 0.44              |
| 42:RW:1:MET:CE    | 42:RW:2:GLU:H     | 2.31                     | 0.44              |
| 42:RW:29:LEU:HD11 | 42:RW:55:ALA:HB2  | 1.98                     | 0.44              |
| 43:RX:70:LEU:HD23 | 43:RX:70:LEU:H    | 1.77                     | 0.44              |
| 47:R1:54:ALA:O    | 47:R1:55:GLY:O    | 2.35                     | 0.44              |
| 47:R1:94:LEU:O    | 47:R1:95:LEU:HB2  | 2.18                     | 0.44              |
| 48:R2:41:ILE:HD12 | 48:R2:41:ILE:O    | 2.16                     | 0.44              |
| 50:R4:15:ILE:N    | 50:R4:15:ILE:CD1  | 2.78                     | 0.44              |
| 50:R4:35:VAL:C    | 50:R4:37:SER:H    | 2.19                     | 0.44              |
| 50:R4:68:ARG:HH11 | 50:R4:69:LYS:HG2  | 1.82                     | 0.44              |
| 1:XA:486:U:H2'    | 1:XA:487:A:C8     | 2.51                     | 0.44              |
| 1:XA:562:C:H4'    | 1:XA:563:A:O5'    | 2.18                     | 0.44              |
| 1:XA:644:G:H4'    | 8:XH:92:ARG:HH21  | 1.82                     | 0.44              |
| 1:XA:1356:G:H2'   | 1:XA:1357:A:C8    | 2.53                     | 0.44              |
| 2:XB:189:ASP:OD2  | 2:XB:205:ASP:OD1  | 2.35                     | 0.44              |
| 4:XD:49:ARG:O     | 4:XD:50:ARG:C     | 2.60                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:XD:76:ARG:O     | 4:XD:79:PHE:HB3   | 2.17                     | 0.44              |
| 4:XD:94:LEU:O     | 4:XD:98:GLU:N     | 2.50                     | 0.44              |
| 9:XI:13:ALA:HB2   | 9:XI:68:GLY:CA    | 2.47                     | 0.44              |
| 9:XI:118:LYS:O    | 9:XI:119:ALA:CB   | 2.65                     | 0.44              |
| 10:XJ:61:GLU:CG   | 14:XN:58:LYS:HE2  | 2.47                     | 0.44              |
| 13:XM:4:ILE:O     | 13:XM:5:ALA:C     | 2.60                     | 0.44              |
| 25:YA:277:C:H3'   | 25:YA:278:A:C5'   | 2.47                     | 0.44              |
| 25:YA:330:A:O2'   | 25:YA:331:A:H8    | 2.01                     | 0.44              |
| 25:YA:539:G:H5'   | 25:YA:540:G:OP2   | 2.18                     | 0.44              |
| 25:YA:878:A:N6    | 25:YA:899:A:O2'   | 2.51                     | 0.44              |
| 25:YA:2151:G:H2'  | 25:YA:2152:G:C8   | 2.53                     | 0.44              |
| 25:YA:2310:A:N6   | 30:YG:79:ASN:HB2  | 2.32                     | 0.44              |
| 25:YA:2620:C:H2'  | 25:YA:2621:A:O4'  | 2.17                     | 0.44              |
| 27:YD:166:GLN:HA  | 27:YD:166:GLN:NE2 | 2.32                     | 0.44              |
| 28:YE:50:GLY:CA   | 28:YE:74:PRO:HG3  | 2.46                     | 0.44              |
| 28:YE:121:ASN:O   | 28:YE:122:PHE:C   | 2.57                     | 0.44              |
| 30:YG:16:ARG:CZ   | 30:YG:31:VAL:HG11 | 2.47                     | 0.44              |
| 30:YG:19:LEU:HA   | 30:YG:22:ARG:HB2  | 1.99                     | 0.44              |
| 30:YG:63:ILE:HG12 | 30:YG:64:THR:N    | 2.33                     | 0.44              |
| 31:YH:6:ARG:C     | 31:YH:8:PRO:CD    | 2.89                     | 0.44              |
| 34:YO:40:VAL:CG1  | 34:YO:41:ALA:N    | 2.80                     | 0.44              |
| 34:YO:120:GLU:OE1 | 39:YT:67:SER:OG   | 2.24                     | 0.44              |
| 35:YP:6:LEU:N     | 35:YP:6:LEU:HD22  | 2.31                     | 0.44              |
| 37:YR:84:ALA:O    | 37:YR:85:PRO:C    | 2.59                     | 0.44              |
| 40:YU:57:PHE:O    | 40:YU:59:ARG:N    | 2.50                     | 0.44              |
| 42:YW:74:ALA:C    | 42:YW:75:TYR:HD1  | 2.25                     | 0.44              |
| 45:YZ:53:ILE:HA   | 45:YZ:71:VAL:HG13 | 1.99                     | 0.44              |
| 47:Y1:60:PHE:HE2  | 47:Y1:91:LYS:NZ   | 2.15                     | 0.44              |
| 48:Y2:41:ILE:HD12 | 48:Y2:41:ILE:O    | 2.16                     | 0.44              |
| 50:Y4:15:ILE:CG2  | 50:Y4:20:ASN:ND2  | 2.81                     | 0.44              |
| 50:Y4:33:VAL:CG1  | 50:Y4:34:GLU:N    | 2.80                     | 0.44              |
| 1:QA:177:C:H2'    | 1:QA:178:C:C6     | 2.52                     | 0.44              |
| 1:QA:186(F):C:H2' | 1:QA:187:C:O4'    | 2.18                     | 0.44              |
| 1:QA:614:A:OP1    | 4:QD:86:LYS:HE3   | 2.17                     | 0.44              |
| 1:QA:667:G:H4'    | 15:QO:51:HIS:CE1  | 2.51                     | 0.44              |
| 1:QA:745:C:OP1    | 1:QA:851:G:O2'    | 2.35                     | 0.44              |
| 1:QA:760:G:O2'    | 17:QQ:98:LEU:HD23 | 2.17                     | 0.44              |
| 1:QA:1190:G:OP1   | 3:QC:5:ILE:HD12   | 2.18                     | 0.44              |
| 1:QA:1278:U:H5''  | 1:QA:1279:A:O4'   | 2.18                     | 0.44              |
| 1:QA:1384:C:H2'   | 1:QA:1385:G:H8    | 1.83                     | 0.44              |
| 2:QB:29:ALA:O     | 2:QB:32:ILE:HG22  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:77:ALA:HB2    | 2:QB:211:ILE:HG21  | 1.99                     | 0.44              |
| 3:QC:22:TRP:HB3    | 3:QC:59:ARG:HB2    | 1.99                     | 0.44              |
| 3:QC:42:LEU:HD12   | 3:QC:45:LYS:NZ     | 2.32                     | 0.44              |
| 3:QC:140:ARG:HH11  | 3:QC:140:ARG:CG    | 2.30                     | 0.44              |
| 4:QD:76:ARG:O      | 4:QD:79:PHE:HB3    | 2.17                     | 0.44              |
| 4:QD:122:ARG:HA    | 4:QD:134:ASP:HB2   | 2.00                     | 0.44              |
| 6:QF:3:ARG:HG2     | 6:QF:93:SER:OG     | 2.17                     | 0.44              |
| 6:QF:76:ALA:HB1    | 6:QF:80:ARG:HH21   | 1.82                     | 0.44              |
| 7:QG:15:ASP:HB3    | 7:QG:20:ASP:N      | 2.15                     | 0.44              |
| 7:QG:45:ASP:O      | 7:QG:49:ILE:HG12   | 2.17                     | 0.44              |
| 11:QK:17:GLY:CA    | 11:QK:77:MET:HE1   | 2.25                     | 0.44              |
| 12:QL:120:TYR:O    | 12:QL:121:GLY:O    | 2.36                     | 0.44              |
| 17:QQ:78:GLU:O     | 17:QQ:79:SER:C     | 2.61                     | 0.44              |
| 20:QT:48:LYS:HB3   | 20:QT:51:GLU:CG    | 2.48                     | 0.44              |
| 25:RA:1491:G:O2'   | 27:RD:101:GLU:HB2  | 2.18                     | 0.44              |
| 25:RA:1588:C:H2'   | 25:RA:1589:C:C6    | 2.52                     | 0.44              |
| 25:RA:1593:G:H3'   | 25:RA:1594:G:H8    | 1.83                     | 0.44              |
| 25:RA:2206:C:H2'   | 25:RA:2207:C:H6    | 1.83                     | 0.44              |
| 25:RA:2396:G:OP1   | 47:R1:25:LYS:NZ    | 2.50                     | 0.44              |
| 25:RA:2875:C:H4'   | 39:RT:5:ALA:HB2    | 1.99                     | 0.44              |
| 27:RD:155:LEU:N    | 27:RD:155:LEU:HD12 | 2.32                     | 0.44              |
| 28:RE:4:ILE:HG12   | 28:RE:91:VAL:HG11  | 1.99                     | 0.44              |
| 29:RF:117:ARG:NH2  | 29:RF:189:THR:O    | 2.50                     | 0.44              |
| 29:RF:132:VAL:HG23 | 29:RF:133:ASN:H    | 1.82                     | 0.44              |
| 29:RF:174:VAL:CG1  | 29:RF:174:VAL:O    | 2.65                     | 0.44              |
| 31:RH:84:SER:OG    | 31:RH:85:LYS:N     | 2.51                     | 0.44              |
| 33:RN:67:LEU:HA    | 33:RN:87:LEU:HD13  | 2.00                     | 0.44              |
| 40:RU:92:ARG:HD2   | 41:RV:11:GLN:CD    | 2.43                     | 0.44              |
| 41:RV:61:VAL:O     | 41:RV:61:VAL:HG22  | 2.16                     | 0.44              |
| 44:RY:88:LYS:HB3   | 44:RY:90:LEU:CD2   | 2.48                     | 0.44              |
| 44:RY:95:LYS:HB2   | 44:RY:99:CYS:O     | 2.18                     | 0.44              |
| 47:R1:10:LYS:HD2   | 47:R1:66:HIS:HE1   | 1.82                     | 0.44              |
| 50:R4:15:ILE:CG2   | 50:R4:20:ASN:ND2   | 2.81                     | 0.44              |
| 52:R6:17:LYS:O     | 52:R6:18:ARG:CB    | 2.64                     | 0.44              |
| 1:XA:236:G:H5''    | 17:XQ:42:TYR:OH    | 2.18                     | 0.44              |
| 1:XA:668:G:O2'     | 15:XO:46:HIS:HB3   | 2.17                     | 0.44              |
| 1:XA:1224:G:O6     | 1:XA:1322:C:H1'    | 2.16                     | 0.44              |
| 3:XC:108:ASN:HB3   | 3:XC:111:LEU:HD12  | 1.99                     | 0.44              |
| 4:XD:96:LEU:C      | 4:XD:98:GLU:N      | 2.72                     | 0.44              |
| 4:XD:132:ARG:HG2   | 4:XD:132:ARG:HH11  | 1.83                     | 0.44              |
| 6:XF:27:GLN:HG2    | 6:XF:27:GLN:H      | 1.65                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:38:LEU:O      | 7:XG:42:ILE:HG13   | 2.17                     | 0.44              |
| 8:XH:110:ALA:HB3   | 8:XH:121:ASP:HB3   | 1.99                     | 0.44              |
| 9:XI:4:TYR:CZ      | 9:XI:88:TYR:HB2    | 2.52                     | 0.44              |
| 10:XJ:100:THR:O    | 10:XJ:101:VAL:HB   | 2.17                     | 0.44              |
| 11:XK:13:GLN:HG3   | 11:XK:75:TYR:CA    | 2.48                     | 0.44              |
| 16:XP:72:ARG:HD3   | 16:XP:72:ARG:O     | 2.18                     | 0.44              |
| 16:XP:72:ARG:CD    | 16:XP:73:LEU:HD23  | 2.48                     | 0.44              |
| 20:XT:89:ARG:HH12  | 20:XT:106:ALA:HB1  | 1.82                     | 0.44              |
| 25:YA:534:U:H2'    | 25:YA:535:C:C6     | 2.52                     | 0.44              |
| 25:YA:971:C:H2'    | 25:YA:972:G:O4'    | 2.18                     | 0.44              |
| 25:YA:1127:A:N1    | 25:YA:2463:C:O2'   | 2.48                     | 0.44              |
| 25:YA:1659:U:O2'   | 25:YA:2712(A):A:N1 | 2.47                     | 0.44              |
| 25:YA:1803:A:O2'   | 27:YD:259:THR:HG21 | 2.17                     | 0.44              |
| 26:YB:113:C:HO2'   | 38:YS:46:VAL:HG13  | 1.82                     | 0.44              |
| 27:YD:80:ALA:O     | 27:YD:113:VAL:HG13 | 2.17                     | 0.44              |
| 29:YF:65:TRP:HZ3   | 29:YF:73:ALA:C     | 2.26                     | 0.44              |
| 29:YF:201:VAL:HG13 | 29:YF:202:PHE:N    | 2.33                     | 0.44              |
| 30:YG:110:ALA:C    | 30:YG:112:PRO:HD2  | 2.42                     | 0.44              |
| 31:YH:6:ARG:CG     | 31:YH:7:LEU:N      | 2.81                     | 0.44              |
| 33:YN:63:THR:HG23  | 33:YN:66:LYS:HE3   | 2.00                     | 0.44              |
| 35:YP:115:LEU:CB   | 35:YP:131:SER:HB2  | 2.47                     | 0.44              |
| 38:YS:56:LEU:O     | 38:YS:57:LYS:O     | 2.36                     | 0.44              |
| 39:YT:80:SER:HA    | 39:YT:81:PRO:HD3   | 1.73                     | 0.44              |
| 42:YW:28:SER:O     | 42:YW:30:GLU:N     | 2.51                     | 0.44              |
| 45:YZ:127:LYS:HB3  | 45:YZ:162:GLU:HG3  | 1.98                     | 0.44              |
| 46:Y0:25:ARG:HA    | 46:Y0:29:GLN:HE22  | 1.83                     | 0.44              |
| 1:QA:1336:C:H1'    | 1:QA:1337:G:C2     | 2.53                     | 0.44              |
| 2:QB:51:LEU:O      | 2:QB:55:PHE:HD2    | 2.00                     | 0.44              |
| 2:QB:207:ALA:C     | 2:QB:209:ARG:N     | 2.76                     | 0.44              |
| 4:QD:206:PHE:CD2   | 4:QD:207:TYR:CE1   | 3.06                     | 0.44              |
| 5:QE:27:ARG:C      | 5:QE:28:PHE:CD1    | 2.96                     | 0.44              |
| 5:QE:78:HIS:HB3    | 8:QH:104:ARG:O     | 2.18                     | 0.44              |
| 5:QE:147:ASP:OD2   | 5:QE:147:ASP:N     | 2.50                     | 0.44              |
| 7:QG:140:ASP:HA    | 7:QG:143:ARG:HH11  | 1.79                     | 0.44              |
| 9:QI:4:TYR:CZ      | 9:QI:88:TYR:HB2    | 2.51                     | 0.44              |
| 9:QI:47:LEU:HD22   | 9:QI:47:LEU:H      | 1.81                     | 0.44              |
| 10:QJ:70:ARG:HH11  | 10:QJ:70:ARG:HG3   | 1.83                     | 0.44              |
| 12:QL:117:ARG:NH2  | 12:QL:124:LYS:HD3  | 2.32                     | 0.44              |
| 12:QL:120:TYR:N    | 12:QL:120:TYR:CD1  | 2.86                     | 0.44              |
| 13:QM:101:GLN:HE21 | 13:QM:101:GLN:HB2  | 1.66                     | 0.44              |
| 15:QO:55:GLY:HA2   | 15:QO:58:MET:HE2   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:QP:15:PRO:O     | 16:QP:16:HIS:ND1   | 2.51                     | 0.44              |
| 20:QT:59:ALA:C     | 20:QT:61:SER:N     | 2.75                     | 0.44              |
| 25:RA:1217:C:OP1   | 40:RU:15:LYS:NZ    | 2.39                     | 0.44              |
| 25:RA:1274:A:N3    | 25:RA:1297:C:H1'   | 2.33                     | 0.44              |
| 25:RA:2313:C:H2'   | 25:RA:2314:C:C6    | 2.53                     | 0.44              |
| 26:RB:70:C:H42     | 26:RB:106:G:H1     | 1.66                     | 0.44              |
| 28:RE:143:ASN:ND2  | 28:RE:143:ASN:N    | 2.65                     | 0.44              |
| 33:RN:7:LYS:HD3    | 33:RN:9:VAL:H      | 1.81                     | 0.44              |
| 33:RN:20:GLY:HA2   | 33:RN:61:ARG:HD2   | 1.99                     | 0.44              |
| 33:RN:57:ALA:O     | 33:RN:124:ALA:HA   | 2.18                     | 0.44              |
| 35:RP:45:LEU:N     | 35:RP:45:LEU:HD12  | 2.32                     | 0.44              |
| 35:RP:144:GLU:N    | 35:RP:144:GLU:CD   | 2.75                     | 0.44              |
| 40:RU:5:LYS:C      | 40:RU:7:GLY:N      | 2.75                     | 0.44              |
| 41:RV:35:LEU:HD22  | 41:RV:35:LEU:N     | 2.23                     | 0.44              |
| 42:RW:74:ALA:C     | 42:RW:75:TYR:HD1   | 2.25                     | 0.44              |
| 42:RW:88:ARG:HH11  | 42:RW:88:ARG:HG2   | 1.82                     | 0.44              |
| 43:RX:87:GLN:HE21  | 43:RX:87:GLN:HB2   | 1.55                     | 0.44              |
| 45:RZ:61:LEU:HB2   | 45:RZ:65:GLN:HB2   | 2.00                     | 0.44              |
| 45:RZ:165:VAL:HG11 | 45:RZ:169:GLU:HB2  | 1.98                     | 0.44              |
| 1:XA:690:G:C6      | 1:XA:691:G:C6      | 3.05                     | 0.44              |
| 1:XA:836:G:OP1     | 18:XR:61:LYS:NZ    | 2.46                     | 0.44              |
| 1:XA:1008:C:N4     | 1:XA:1021:G:H1     | 2.14                     | 0.44              |
| 1:XA:1070:U:H2'    | 1:XA:1071:C:H6     | 1.83                     | 0.44              |
| 2:XB:54:THR:HG21   | 2:XB:201:ILE:HD11  | 1.99                     | 0.44              |
| 3:XC:140:ARG:HH11  | 3:XC:140:ARG:CG    | 2.30                     | 0.44              |
| 4:XD:199:ASN:C     | 4:XD:201:GLN:H     | 2.25                     | 0.44              |
| 10:XJ:38:ILE:CG1   | 10:XJ:71:LEU:HB3   | 2.48                     | 0.44              |
| 10:XJ:62:HIS:N     | 10:XJ:62:HIS:CD2   | 2.85                     | 0.44              |
| 11:XK:121:PRO:HD2  | 11:XK:126:ARG:CD   | 2.46                     | 0.44              |
| 13:XM:16:ASP:O     | 13:XM:19:LEU:HD23  | 2.17                     | 0.44              |
| 13:XM:50:GLU:OE1   | 50:Y4:32:TYR:CE2   | 2.70                     | 0.44              |
| 16:XP:50:LYS:HD3   | 16:XP:50:LYS:O     | 2.17                     | 0.44              |
| 17:XQ:66:SER:O     | 17:XQ:67:LYS:C     | 2.61                     | 0.44              |
| 18:XR:82:THR:HG22  | 18:XR:83:GLU:H     | 1.80                     | 0.44              |
| 25:YA:307:G:H21    | 25:YA:330:A:N6     | 2.15                     | 0.44              |
| 25:YA:414:C:O2     | 25:YA:1864:U:O2'   | 2.34                     | 0.44              |
| 25:YA:2015:A:C1'   | 51:Y5:2:ALA:HA     | 2.32                     | 0.44              |
| 25:YA:2645:G:H3'   | 25:YA:2646:C:H5'   | 1.99                     | 0.44              |
| 28:YE:172:VAL:HG13 | 28:YE:182:LEU:HD11 | 1.98                     | 0.44              |
| 29:YF:111:ALA:O    | 29:YF:112:MET:C    | 2.59                     | 0.44              |
| 29:YF:149:ASP:OD2  | 29:YF:151:SER:HB3  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:YG:51:ARG:HB3  | 30:YG:51:ARG:NH1  | 2.33                     | 0.44              |
| 33:YN:109:LYS:H   | 33:YN:109:LYS:CD  | 2.26                     | 0.44              |
| 36:YQ:60:ARG:HB2  | 36:YQ:60:ARG:HH21 | 1.82                     | 0.44              |
| 38:YS:110:LEU:HA  | 38:YS:112:PHE:CE1 | 2.52                     | 0.44              |
| 38:YS:110:LEU:HA  | 38:YS:112:PHE:CZ  | 2.53                     | 0.44              |
| 40:YU:27:LEU:O    | 40:YU:28:ARG:C    | 2.60                     | 0.44              |
| 40:YU:86:ALA:CB   | 40:YU:88:ILE:HD11 | 2.48                     | 0.44              |
| 41:YV:35:LEU:C    | 41:YV:37:VAL:N    | 2.75                     | 0.44              |
| 41:YV:72:VAL:HG13 | 41:YV:85:LYS:HB3  | 2.00                     | 0.44              |
| 42:YW:1:MET:CE    | 42:YW:2:GLU:H     | 2.31                     | 0.44              |
| 50:Y4:35:VAL:C    | 50:Y4:37:SER:H    | 2.19                     | 0.44              |
| 54:Y8:47:LYS:HD2  | 54:Y8:48:PHE:N    | 2.33                     | 0.44              |
| 2:QB:192:SER:OG   | 2:QB:193:ASP:N    | 2.51                     | 0.44              |
| 3:QC:69:HIS:N     | 3:QC:69:HIS:ND1   | 2.66                     | 0.44              |
| 4:QD:60:GLU:HG2   | 4:QD:202:LEU:HD12 | 2.00                     | 0.44              |
| 5:QE:90:VAL:C     | 5:QE:91:LEU:HD12  | 2.42                     | 0.44              |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:N    | 2.32                     | 0.44              |
| 13:QM:90:LEU:HD12 | 13:QM:91:ARG:N    | 2.33                     | 0.44              |
| 16:QP:47:ASP:C    | 16:QP:49:LEU:N    | 2.75                     | 0.44              |
| 25:RA:954:G:OP1   | 36:RQ:15:GLY:N    | 2.41                     | 0.44              |
| 25:RA:2396:G:H1'  | 47:R1:30:VAL:HG13 | 1.99                     | 0.44              |
| 25:RA:2469:A:H4'  | 25:RA:2469:A:OP1  | 2.17                     | 0.44              |
| 26:RB:43:C:O2     | 30:RG:93:THR:HB   | 2.17                     | 0.44              |
| 27:RD:30:GLU:HG3  | 27:RD:63:ARG:NE   | 2.32                     | 0.44              |
| 27:RD:52:ARG:HB2  | 27:RD:53:PHE:CD2  | 2.53                     | 0.44              |
| 27:RD:95:LEU:HD12 | 27:RD:95:LEU:O    | 2.17                     | 0.44              |
| 30:RG:180:PHE:C   | 30:RG:182:LYS:N   | 2.76                     | 0.44              |
| 33:RN:96:GLU:CG   | 33:RN:97:ARG:N    | 2.72                     | 0.44              |
| 34:RO:77:ILE:O    | 34:RO:77:ILE:HG23 | 2.17                     | 0.44              |
| 34:RO:92:GLU:O    | 34:RO:93:PRO:C    | 2.58                     | 0.44              |
| 35:RP:101:VAL:HA  | 35:RP:106:LEU:HB2 | 1.99                     | 0.44              |
| 37:RR:31:HIS:C    | 37:RR:33:ARG:H    | 2.25                     | 0.44              |
| 37:RR:79:LEU:HD23 | 37:RR:79:LEU:O    | 2.16                     | 0.44              |
| 40:RU:52:ARG:NH1  | 40:RU:52:ARG:CG   | 2.76                     | 0.44              |
| 40:RU:57:PHE:C    | 40:RU:59:ARG:N    | 2.74                     | 0.44              |
| 45:RZ:157:LEU:HA  | 45:RZ:158:PRO:HD2 | 1.72                     | 0.44              |
| 49:R3:50:VAL:HB   | 49:R3:53:LEU:HD12 | 2.00                     | 0.44              |
| 51:R5:52:TYR:CD1  | 51:R5:52:TYR:N    | 2.85                     | 0.44              |
| 1:XA:156:G:H2'    | 1:XA:157:G:H8     | 1.82                     | 0.44              |
| 1:XA:173:U:H5''   | 1:XA:197:A:O4'    | 2.18                     | 0.44              |
| 1:XA:361:G:H2'    | 1:XA:362:G:O4'    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:502:G:OP1     | 12:XL:118:SER:N    | 2.41                     | 0.44              |
| 2:XB:24:TRP:CD2    | 2:XB:26:PRO:HD3    | 2.52                     | 0.44              |
| 2:XB:178:ARG:NH2   | 8:XH:74:PRO:CB     | 2.77                     | 0.44              |
| 3:XC:43:LEU:HD11   | 3:XC:66:VAL:HG11   | 1.98                     | 0.44              |
| 3:XC:188:LEU:HD12  | 3:XC:195:VAL:CG1   | 2.48                     | 0.44              |
| 5:XE:48:ALA:HB2    | 5:XE:57:LYS:HD3    | 2.00                     | 0.44              |
| 6:XF:35:ALA:HA     | 6:XF:67:MET:HB3    | 1.99                     | 0.44              |
| 8:XH:28:ALA:O      | 8:XH:29:SER:HB2    | 2.18                     | 0.44              |
| 10:XJ:33:GLN:HB2   | 10:XJ:75:ILE:HD11  | 1.99                     | 0.44              |
| 11:XK:83:ILE:HG12  | 11:XK:109:VAL:HG23 | 1.99                     | 0.44              |
| 11:XK:106:LYS:O    | 11:XK:107:SER:CB   | 2.65                     | 0.44              |
| 14:YN:24:CYS:HB3   | 14:YN:28:GLY:H     | 1.83                     | 0.44              |
| 16:XP:68:ASP:C     | 16:XP:70:ALA:N     | 2.75                     | 0.44              |
| 17:XQ:41:LYS:HZ1   | 17:XQ:92:ARG:HH22  | 1.65                     | 0.44              |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6  | 2.53                     | 0.44              |
| 25:YA:330:A:C2     | 25:YA:1210:A:H2'   | 2.51                     | 0.44              |
| 25:YA:660:G:O3'    | 29:YF:38:ARG:NH2   | 2.50                     | 0.44              |
| 25:YA:666:G:H4'    | 35:YP:49:ARG:HH12  | 1.79                     | 0.44              |
| 25:YA:859:G:H5'    | 25:YA:2268:A:O2'   | 2.17                     | 0.44              |
| 25:YA:1266:G:N7    | 42:YW:15:ARG:NH1   | 2.65                     | 0.44              |
| 25:YA:2208:U:C1'   | 27:YD:151:LYS:HE2  | 2.47                     | 0.44              |
| 25:YA:2639:A:H1'   | 25:YA:2778:A:C2    | 2.53                     | 0.44              |
| 25:YA:2702:U:HO2'  | 25:YA:2703:C:H6    | 1.61                     | 0.44              |
| 27:YD:44:ASN:HB2   | 27:YD:49:ILE:HA    | 1.93                     | 0.44              |
| 28:YE:1:MET:HE2    | 28:YE:1:MET:H1     | 1.83                     | 0.44              |
| 28:YE:93:VAL:C     | 28:YE:95:ILE:N     | 2.75                     | 0.44              |
| 28:YE:120:TRP:CE3  | 28:YE:155:LYS:HD3  | 2.53                     | 0.44              |
| 31:YH:153:LYS:HG3  | 31:YH:162:ILE:H    | 1.78                     | 0.44              |
| 32:YI:49:ALA:HA    | 32:YI:52:ARG:HG2   | 1.99                     | 0.44              |
| 33:YN:131:GLN:CD   | 33:YN:132:ALA:N    | 2.74                     | 0.44              |
| 35:YP:45:LEU:N     | 35:YP:45:LEU:HD12  | 2.33                     | 0.44              |
| 35:YP:107:LYS:HB2  | 35:YP:110:TYR:HD2  | 1.83                     | 0.44              |
| 40:YU:97:ASP:HA    | 40:YU:100:VAL:CG2  | 2.47                     | 0.44              |
| 46:Y0:25:ARG:HD2   | 46:Y0:29:GLN:NE2   | 2.33                     | 0.44              |
| 49:Y3:60:GLU:HG2   | 49:Y3:60:GLU:O     | 2.16                     | 0.44              |
| 50:Y4:23:GLU:O     | 50:Y4:24:THR:OG1   | 2.34                     | 0.44              |
| 50:Y4:39:CYS:HB3   | 50:Y4:41:PRO:HD2   | 2.00                     | 0.44              |
| 1:QA:475:G:H2'     | 1:QA:476:G:C8      | 2.53                     | 0.44              |
| 1:QA:690:G:H22     | 11:QK:55:LYS:HZ2   | 1.66                     | 0.44              |
| 1:QA:770:C:H2'     | 1:QA:771:G:H8      | 1.82                     | 0.44              |
| 1:QA:1002:G:H1     | 1:QA:1038:C:H42    | 1.64                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8  | 2.52                     | 0.44              |
| 1:QA:1063:C:H2'    | 1:QA:1064:G:C8     | 2.53                     | 0.44              |
| 1:QA:1322:C:O2     | 1:QA:1322:C:H2'    | 2.16                     | 0.44              |
| 2:QB:229:VAL:O     | 2:QB:229:VAL:HG12  | 2.18                     | 0.44              |
| 5:QE:67:VAL:HG22   | 5:QE:68:GLU:N      | 2.33                     | 0.44              |
| 5:QE:101:ILE:HD13  | 5:QE:101:ILE:H     | 1.82                     | 0.44              |
| 7:QG:62:PHE:O      | 7:QG:64:GLN:N      | 2.51                     | 0.44              |
| 8:QH:16:ALA:HB2    | 8:QH:24:THR:CG2    | 2.45                     | 0.44              |
| 9:QI:5:TYR:CD2     | 9:QI:6:GLY:N       | 2.86                     | 0.44              |
| 9:QI:13:ALA:HB2    | 9:QI:68:GLY:CA     | 2.47                     | 0.44              |
| 9:QI:100:GLY:C     | 9:QI:102:LEU:H     | 2.26                     | 0.44              |
| 10:QJ:54:PHE:CD2   | 10:QJ:55:LYS:HD2   | 2.52                     | 0.44              |
| 11:QK:88:GLY:O     | 11:QK:89:ALA:C     | 2.61                     | 0.44              |
| 15:QO:10:LYS:O     | 15:QO:14:GLU:HB2   | 2.18                     | 0.44              |
| 16:QP:83:GLU:HG3   | 16:QP:84:ALA:N     | 2.33                     | 0.44              |
| 18:QR:20:ALA:O     | 18:QR:21:LYS:HG3   | 2.18                     | 0.44              |
| 25:RA:103:A:OP2    | 25:RA:103:A:C8     | 2.70                     | 0.44              |
| 25:RA:242:G:O3'    | 54:R8:6:THR:HG23   | 2.18                     | 0.44              |
| 25:RA:1651:G:H2'   | 25:RA:1652:A:O4'   | 2.18                     | 0.44              |
| 25:RA:1655:A:O3'   | 28:RE:115:GLY:HA3  | 2.17                     | 0.44              |
| 25:RA:2168:G:H2'   | 25:RA:2168:G:N3    | 2.33                     | 0.44              |
| 25:RA:2375:G:O2'   | 25:RA:2377:A:N7    | 2.46                     | 0.44              |
| 25:RA:2740:A:C6    | 25:RA:2741:A:C6    | 3.06                     | 0.44              |
| 27:RD:12:SER:O     | 27:RD:14:ARG:N     | 2.51                     | 0.44              |
| 27:RD:214:TRP:C    | 27:RD:216:GLY:H    | 2.25                     | 0.44              |
| 28:RE:95:ILE:HG22  | 28:RE:95:ILE:O     | 2.16                     | 0.44              |
| 29:RF:65:TRP:CZ2   | 29:RF:72:ARG:NH2   | 2.86                     | 0.44              |
| 29:RF:79:GLY:O     | 29:RF:80:ALA:C     | 2.61                     | 0.44              |
| 29:RF:109:GLY:O    | 29:RF:110:LEU:C    | 2.58                     | 0.44              |
| 30:RG:129:GLY:HA2  | 30:RG:169:ALA:HB2  | 1.99                     | 0.44              |
| 32:RI:99:GLU:OE2   | 32:RI:103:ARG:NH2  | 2.28                     | 0.44              |
| 33:RN:65:LYS:O     | 33:RN:66:LYS:C     | 2.60                     | 0.44              |
| 34:RO:91:LEU:N     | 34:RO:91:LEU:CD2   | 2.80                     | 0.44              |
| 35:RP:83:VAL:HG11  | 35:RP:112:LEU:HD21 | 1.97                     | 0.44              |
| 40:RU:57:PHE:O     | 40:RU:58:ARG:C     | 2.59                     | 0.44              |
| 44:RY:97:ARG:HG2   | 44:RY:97:ARG:HH11  | 1.82                     | 0.44              |
| 47:R1:8:SER:CB     | 47:R1:66:HIS:CE1   | 3.01                     | 0.44              |
| 52:R6:34:LEU:O     | 52:R6:36:LEU:HD22  | 2.17                     | 0.44              |
| 53:R7:48:LYS:CG    | 53:R7:49:ARG:H     | 2.23                     | 0.44              |
| 1:XA:373:A:H61     | 1:XA:391:G:H1'     | 1.82                     | 0.44              |
| 1:XA:411:A:N6      | 1:XA:413:G:H21     | 2.11                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:986:A:H2'    | 1:XA:987:G:C8      | 2.53                     | 0.44              |
| 1:XA:1159:U:O2'   | 1:XA:1160:G:N7     | 2.51                     | 0.44              |
| 1:XA:1187:G:P     | 9:XI:113:LYS:NZ    | 2.91                     | 0.44              |
| 2:XB:30:ARG:HH21  | 2:XB:194:PRO:HG2   | 1.82                     | 0.44              |
| 2:XB:192:SER:OG   | 2:XB:193:ASP:N     | 2.50                     | 0.44              |
| 3:XC:68:VAL:HG12  | 3:XC:70:VAL:HG23   | 1.98                     | 0.44              |
| 4:XD:9:CYS:SG     | 4:XD:32:ALA:HB2    | 2.58                     | 0.44              |
| 4:XD:33:MET:HE1   | 4:XD:37:PRO:O      | 2.18                     | 0.44              |
| 5:XE:94:ALA:HB2   | 5:XE:119:LEU:HG    | 2.00                     | 0.44              |
| 8:XH:6:ILE:HB     | 8:XH:85:ARG:HH11   | 1.74                     | 0.44              |
| 13:XM:3:ARG:C     | 13:XM:9:ILE:HG21   | 2.43                     | 0.44              |
| 15:XO:29:VAL:HB   | 15:XO:81:LEU:HD21  | 1.99                     | 0.44              |
| 16:XP:15:PRO:O    | 16:XP:16:HIS:ND1   | 2.51                     | 0.44              |
| 19:XS:3:ARG:CG    | 19:XS:4:SER:H      | 2.21                     | 0.44              |
| 25:YA:628:G:H2'   | 25:YA:629:G:H8     | 1.83                     | 0.44              |
| 25:YA:680:G:H2'   | 25:YA:681:G:H8     | 1.81                     | 0.44              |
| 25:YA:691:C:H2'   | 25:YA:692:C:C6     | 2.52                     | 0.44              |
| 25:YA:1240:U:O2'  | 25:YA:1241:A:H5'   | 2.17                     | 0.44              |
| 25:YA:1338:G:N7   | 43:YX:62:LYS:NZ    | 2.56                     | 0.44              |
| 27:YD:17:THR:HG21 | 27:YD:204:ILE:HA   | 1.99                     | 0.44              |
| 27:YD:44:ASN:CB   | 27:YD:49:ILE:HG22  | 2.46                     | 0.44              |
| 27:YD:102:LYS:O   | 27:YD:103:ARG:CG   | 2.66                     | 0.44              |
| 27:YD:143:HIS:HD2 | 27:YD:144:ALA:HB2  | 1.82                     | 0.44              |
| 27:YD:145:VAL:HB  | 27:YD:155:LEU:HB2  | 1.99                     | 0.44              |
| 27:YD:155:LEU:N   | 27:YD:155:LEU:HD12 | 2.32                     | 0.44              |
| 28:YE:2:LYS:HG2   | 28:YE:95:ILE:HG22  | 1.99                     | 0.44              |
| 28:YE:48:GLN:HE21 | 28:YE:48:GLN:HB3   | 1.55                     | 0.44              |
| 29:YF:184:TYR:CE2 | 29:YF:188:ARG:HD2  | 2.52                     | 0.44              |
| 30:YG:16:ARG:NH2  | 30:YG:31:VAL:CG1   | 2.75                     | 0.44              |
| 32:YI:3:VAL:HG12  | 32:YI:38:LEU:HA    | 1.98                     | 0.44              |
| 33:YN:112:LEU:C   | 33:YN:114:ARG:O    | 2.61                     | 0.44              |
| 34:YO:47:ILE:HG13 | 34:YO:48:PRO:HD2   | 1.99                     | 0.44              |
| 35:YP:88:LEU:O    | 35:YP:90:ARG:N     | 2.50                     | 0.44              |
| 42:YW:14:PRO:HB3  | 42:YW:18:ARG:HE    | 1.83                     | 0.44              |
| 44:YY:36:ALA:HB1  | 44:YY:67:LEU:O     | 2.16                     | 0.44              |
| 47:Y1:49:VAL:HG12 | 47:Y1:51:VAL:HG23  | 1.99                     | 0.44              |
| 50:Y4:68:ARG:HH11 | 50:Y4:69:LYS:HG2   | 1.82                     | 0.44              |
| 52:Y6:19:ARG:HD2  | 52:Y6:19:ARG:HA    | 1.77                     | 0.44              |
| 1:QA:186(D):C:H2' | 1:QA:186(E):C:C6   | 2.52                     | 0.44              |
| 1:QA:797:C:OP1    | 11:QK:124:LYS:HE2  | 2.18                     | 0.44              |
| 2:QB:47:THR:HG22  | 2:QB:51:LEU:CG     | 2.48                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:132:LYS:HA    | 2:QB:135:GLN:CB    | 2.43                     | 0.44              |
| 5:QE:42:GLY:CA     | 5:QE:136:MET:HE1   | 2.46                     | 0.44              |
| 5:QE:80:ILE:C      | 5:QE:81:GLU:HG2    | 2.43                     | 0.44              |
| 5:QE:152:ARG:HD3   | 8:QH:44:PHE:CE1    | 2.52                     | 0.44              |
| 7:QG:16:LEU:HD13   | 9:QI:45:ALA:HB2    | 1.99                     | 0.44              |
| 8:QH:118:VAL:O     | 8:QH:119:LEU:HD23  | 2.17                     | 0.44              |
| 9:QI:100:GLY:C     | 9:QI:102:LEU:N     | 2.71                     | 0.44              |
| 10:QJ:38:ILE:CG1   | 10:QJ:71:LEU:HB3   | 2.48                     | 0.44              |
| 10:QJ:61:GLU:CG    | 14:QN:58:LYS:HE2   | 2.47                     | 0.44              |
| 12:QL:91:LYS:HE2   | 12:QL:91:LYS:HB2   | 1.76                     | 0.44              |
| 13:QM:53:VAL:HG12  | 13:QM:57:ARG:HH12  | 1.82                     | 0.44              |
| 15:QO:50:HIS:O     | 15:QO:51:HIS:C     | 2.61                     | 0.44              |
| 17:QQ:82:MET:C     | 17:QQ:84:LEU:H     | 2.25                     | 0.44              |
| 17:QQ:92:ARG:HG3   | 17:QQ:92:ARG:NH1   | 2.30                     | 0.44              |
| 20:QT:36:LEU:C     | 20:QT:38:LYS:N     | 2.71                     | 0.44              |
| 25:RA:330:A:H2     | 25:RA:1210:A:H2'   | 1.82                     | 0.44              |
| 25:RA:856:C:O2'    | 25:RA:857:C:OP1    | 2.32                     | 0.44              |
| 25:RA:2041:U:H2'   | 25:RA:2042:A:C8    | 2.52                     | 0.44              |
| 25:RA:2572:A:N7    | 28:RE:145:LYS:HB2  | 2.33                     | 0.44              |
| 27:RD:11:PRO:O     | 27:RD:12:SER:CB    | 2.65                     | 0.44              |
| 27:RD:25:THR:CG2   | 27:RD:25:THR:O     | 2.65                     | 0.44              |
| 27:RD:44:ASN:H     | 27:RD:44:ASN:ND2   | 1.97                     | 0.44              |
| 27:RD:155:LEU:HD23 | 27:RD:177:LEU:HD21 | 2.00                     | 0.44              |
| 27:RD:172:TYR:HD1  | 27:RD:185:VAL:C    | 2.26                     | 0.44              |
| 27:RD:237:GLU:HB3  | 27:RD:238:GLY:H    | 1.49                     | 0.44              |
| 28:RE:11:MET:O     | 28:RE:12:THR:HB    | 2.18                     | 0.44              |
| 28:RE:13:ARG:HH11  | 28:RE:13:ARG:HB3   | 1.82                     | 0.44              |
| 28:RE:199:ARG:HH11 | 28:RE:199:ARG:HG3  | 1.82                     | 0.44              |
| 30:RG:67:LYS:HD2   | 30:RG:67:LYS:N     | 2.33                     | 0.44              |
| 33:RN:114:ARG:O    | 33:RN:115:ARG:CB   | 2.65                     | 0.44              |
| 36:RQ:20:ALA:C     | 36:RQ:21:THR:HG23  | 2.43                     | 0.44              |
| 37:RR:12:ARG:HG3   | 37:RR:12:ARG:NH1   | 2.32                     | 0.44              |
| 37:RR:33:ARG:HA    | 37:RR:114:VAL:O    | 2.18                     | 0.44              |
| 40:RU:79:PHE:CE2   | 40:RU:83:LEU:CD1   | 3.00                     | 0.44              |
| 41:RV:72:VAL:HG13  | 41:RV:85:LYS:HB3   | 2.00                     | 0.44              |
| 43:RX:14:SER:HB2   | 43:RX:15:GLU:OE1   | 2.18                     | 0.44              |
| 44:RY:15:VAL:HB    | 44:RY:20:TYR:O     | 2.17                     | 0.44              |
| 50:R4:33:VAL:CG1   | 50:R4:34:GLU:H     | 2.22                     | 0.44              |
| 50:R4:39:CYS:HB3   | 50:R4:41:PRO:HD2   | 2.00                     | 0.44              |
| 1:XA:577:G:H1'     | 1:XA:816:A:C4      | 2.53                     | 0.44              |
| 1:XA:1124:G:H3'    | 1:XA:1145:C:H41    | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1394:A:OP1   | 1:XA:1394:A:H8    | 2.00                     | 0.44              |
| 1:XA:1427:U:H2'   | 1:XA:1428:A:C8    | 2.52                     | 0.44              |
| 1:XA:1511:G:H2'   | 1:XA:1512:U:O4'   | 2.18                     | 0.44              |
| 3:XC:69:HIS:N     | 3:XC:69:HIS:ND1   | 2.66                     | 0.44              |
| 4:XD:52:SER:HB3   | 4:XD:55:ALA:HB3   | 2.00                     | 0.44              |
| 5:XE:27:ARG:C     | 5:XE:28:PHE:CD1   | 2.96                     | 0.44              |
| 7:XG:69:VAL:O     | 7:XG:69:VAL:CG1   | 2.62                     | 0.44              |
| 7:XG:75:VAL:HG13  | 7:XG:145:ALA:HA   | 2.00                     | 0.44              |
| 8:XH:74:PRO:O     | 8:XH:75:ARG:C     | 2.59                     | 0.44              |
| 8:XH:109:ILE:HD11 | 8:XH:120:THR:HG22 | 2.00                     | 0.44              |
| 10:XJ:51:ARG:HG2  | 10:XJ:51:ARG:NH1  | 2.33                     | 0.44              |
| 12:XL:120:TYR:O   | 12:XL:121:GLY:O   | 2.36                     | 0.44              |
| 13:XM:80:ARG:NH1  | 19:XS:65:ASN:O    | 2.51                     | 0.44              |
| 15:XO:55:GLY:HA2  | 15:XO:58:MET:HE2  | 2.00                     | 0.44              |
| 15:XO:58:MET:O    | 15:XO:59:MET:C    | 2.61                     | 0.44              |
| 19:XS:8:GLY:O     | 19:XS:9:VAL:CG2   | 2.57                     | 0.44              |
| 20:XT:48:LYS:HB3  | 20:XT:51:GLU:CG   | 2.48                     | 0.44              |
| 25:YA:2182:G:H2'  | 25:YA:2183:C:C6   | 2.52                     | 0.44              |
| 25:YA:2311:A:H1'  | 30:YG:82:LEU:HD11 | 1.99                     | 0.44              |
| 25:YA:2334:G:H5'  | 38:YS:9:ARG:HG2   | 2.00                     | 0.44              |
| 27:YD:95:LEU:HD12 | 27:YD:95:LEU:O    | 2.17                     | 0.44              |
| 27:YD:213:ARG:HD2 | 27:YD:213:ARG:HA  | 1.60                     | 0.44              |
| 27:YD:272:ALA:HB1 | 27:YD:273:ARG:H   | 1.58                     | 0.44              |
| 29:YF:24:LEU:HD12 | 29:YF:24:LEU:N    | 2.33                     | 0.44              |
| 29:YF:42:ALA:O    | 29:YF:45:ARG:HB2  | 2.18                     | 0.44              |
| 29:YF:65:TRP:CZ2  | 29:YF:72:ARG:NH2  | 2.86                     | 0.44              |
| 29:YF:108:LYS:O   | 29:YF:109:GLY:C   | 2.61                     | 0.44              |
| 33:YN:67:LEU:HA   | 33:YN:87:LEU:HD13 | 2.00                     | 0.44              |
| 39:YT:99:LEU:CD1  | 39:YT:99:LEU:O    | 2.65                     | 0.44              |
| 40:YU:79:PHE:CE2  | 40:YU:83:LEU:CD1  | 3.01                     | 0.44              |
| 44:YY:15:VAL:HB   | 44:YY:20:TYR:O    | 2.17                     | 0.44              |
| 44:YY:95:LYS:C    | 44:YY:96:ILE:O    | 2.61                     | 0.44              |
| 50:Y4:39:CYS:O    | 50:Y4:40:HIS:CB   | 2.66                     | 0.44              |
| 52:Y6:34:LEU:O    | 52:Y6:36:LEU:HD22 | 2.17                     | 0.44              |
| 1:QA:56:U:H2'     | 1:QA:57:G:C8      | 2.53                     | 0.44              |
| 1:QA:263:A:OP1    | 20:QT:79:ARG:HD3  | 2.17                     | 0.44              |
| 1:QA:565:U:OP2    | 1:QA:566:G:O2'    | 2.31                     | 0.44              |
| 1:QA:921:U:O2'    | 5:QE:19:MET:O     | 2.26                     | 0.44              |
| 1:QA:1084:G:H5'   | 1:QA:1102:A:OP2   | 2.18                     | 0.44              |
| 1:QA:1337:G:H5''  | 1:QA:1338:G:OP1   | 2.18                     | 0.44              |
| 2:QB:17:PHE:CG    | 2:QB:44:LEU:HD11  | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:87:ARG:NH1    | 2:QB:223:ILE:HD12  | 2.33                     | 0.44              |
| 3:QC:129:ALA:C     | 3:QC:131:ARG:N     | 2.72                     | 0.44              |
| 4:QD:146:ILE:H     | 4:QD:146:ILE:CD1   | 2.29                     | 0.44              |
| 8:QH:23:SER:HB3    | 8:QH:62:TYR:HA     | 2.00                     | 0.44              |
| 8:QH:88:LYS:HB3    | 8:QH:89:PRO:HD2    | 2.00                     | 0.44              |
| 8:QH:122:ARG:O     | 8:QH:123:GLU:C     | 2.60                     | 0.44              |
| 11:QK:13:GLN:HG3   | 11:QK:75:TYR:CA    | 2.48                     | 0.44              |
| 11:QK:34:ASP:OD1   | 11:QK:38:ASN:HB2   | 2.18                     | 0.44              |
| 11:QK:106:LYS:O    | 11:QK:107:SER:CB   | 2.65                     | 0.44              |
| 16:QP:72:ARG:CD    | 16:QP:73:LEU:HD23  | 2.48                     | 0.44              |
| 22:QV:4:G:C6       | 22:QV:70:G:N1      | 2.86                     | 0.44              |
| 25:RA:712:G:H1     | 25:RA:719:C:H42    | 1.66                     | 0.44              |
| 25:RA:898:C:C2'    | 25:RA:899:A:H5'    | 2.46                     | 0.44              |
| 25:RA:1093:G:OP1   | 31:RH:170:ARG:HD2  | 2.18                     | 0.44              |
| 25:RA:1210:A:H4'   | 25:RA:1211:U:O5'   | 2.18                     | 0.44              |
| 25:RA:1594:G:H2'   | 25:RA:1595:G:C8    | 2.53                     | 0.44              |
| 25:RA:2242:G:H2'   | 25:RA:2243:U:O4'   | 2.18                     | 0.44              |
| 25:RA:2271:G:OP1   | 46:R0:18:ALA:HB1   | 2.18                     | 0.44              |
| 25:RA:2292:C:H2'   | 25:RA:2293:C:C6    | 2.52                     | 0.44              |
| 25:RA:2863:C:H2'   | 25:RA:2864:G:C8    | 2.53                     | 0.44              |
| 26:RB:89:G:H2'     | 26:RB:89(A):A:C8   | 2.53                     | 0.44              |
| 27:RD:206:LEU:HD23 | 27:RD:206:LEU:HA   | 1.49                     | 0.44              |
| 28:RE:52:LEU:HB2   | 28:RE:75:VAL:CG2   | 2.40                     | 0.44              |
| 29:RF:127:GLU:C    | 29:RF:129:PHE:H    | 2.26                     | 0.44              |
| 30:RG:53:LEU:C     | 30:RG:55:LYS:H     | 2.26                     | 0.44              |
| 31:RH:58:GLU:O     | 31:RH:59:ARG:C     | 2.61                     | 0.44              |
| 31:RH:125:VAL:CG1  | 31:RH:126:PRO:CG   | 2.94                     | 0.44              |
| 34:RO:63:VAL:O     | 34:RO:63:VAL:HG23  | 2.18                     | 0.44              |
| 36:RQ:34:LEU:HB2   | 36:RQ:118:LEU:HD22 | 1.99                     | 0.44              |
| 36:RQ:133:ARG:CG   | 36:RQ:134:ARG:N    | 2.78                     | 0.44              |
| 38:RS:38:GLN:CG    | 38:RS:47:THR:HG21  | 2.48                     | 0.44              |
| 38:RS:78:LEU:HD21  | 38:RS:108:GLY:HA2  | 1.99                     | 0.44              |
| 38:RS:86:ALA:O     | 38:RS:87:PHE:CB    | 2.65                     | 0.44              |
| 38:RS:110:LEU:HA   | 38:RS:112:PHE:CE1  | 2.52                     | 0.44              |
| 39:RT:114:LEU:HD23 | 39:RT:114:LEU:HA   | 1.74                     | 0.44              |
| 42:RW:14:PRO:HB3   | 42:RW:18:ARG:HE    | 1.83                     | 0.44              |
| 43:RX:3:THR:HA     | 43:RX:6:ASP:OD2    | 2.18                     | 0.44              |
| 44:RY:95:LYS:C     | 44:RY:96:ILE:O     | 2.61                     | 0.44              |
| 54:R8:28:GLY:O     | 54:R8:29:LYS:C     | 2.61                     | 0.44              |
| 54:R8:40:GLU:O     | 54:R8:43:GLN:N     | 2.50                     | 0.44              |
| 1:XA:272:C:H2'     | 1:XA:273:A:H8      | 1.82                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1095:U:P      | 1:XA:1108:G:H1    | 2.40                     | 0.44              |
| 2:XB:33:TYR:HD1    | 2:XB:33:TYR:O     | 2.00                     | 0.44              |
| 4:XD:93:PHE:CZ     | 4:XD:97:LEU:HD11  | 2.52                     | 0.44              |
| 5:XE:62:ALA:O      | 5:XE:64:ARG:N     | 2.51                     | 0.44              |
| 5:XE:80:ILE:HG13   | 5:XE:82:VAL:HG23  | 1.99                     | 0.44              |
| 6:XF:3:ARG:HG2     | 6:XF:93:SER:OG    | 2.17                     | 0.44              |
| 7:XG:151:TYR:HE1   | 11:XK:54:ARG:HD3  | 1.83                     | 0.44              |
| 8:XH:23:SER:HB3    | 8:XH:62:TYR:HA    | 2.00                     | 0.44              |
| 8:XH:88:LYS:HB3    | 8:XH:89:PRO:HD2   | 2.00                     | 0.44              |
| 9:XI:10:ARG:NE     | 9:XI:105:ASP:CB   | 2.81                     | 0.44              |
| 9:XI:100:GLY:C     | 9:XI:102:LEU:H    | 2.25                     | 0.44              |
| 17:XQ:13:ASP:O     | 17:XQ:15:MET:N    | 2.50                     | 0.44              |
| 20:XT:28:ALA:O     | 20:XT:30:LYS:N    | 2.50                     | 0.44              |
| 25:YA:976:C:H42    | 25:YA:987:G:H1    | 1.64                     | 0.44              |
| 25:YA:1093:G:H4'   | 31:YH:170:ARG:NH2 | 2.33                     | 0.44              |
| 25:YA:2404:C:O3'   | 35:YP:77:ARG:NH2  | 2.50                     | 0.44              |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:N   | 2.32                     | 0.44              |
| 29:YF:174:VAL:CG1  | 29:YF:174:VAL:O   | 2.65                     | 0.44              |
| 30:YG:67:LYS:CE    | 50:Y4:6:HIS:NE2   | 2.74                     | 0.44              |
| 30:YG:136:ARG:O    | 30:YG:137:GLU:C   | 2.61                     | 0.44              |
| 31:YH:37:VAL:HG11  | 31:YH:68:THR:HG23 | 1.98                     | 0.44              |
| 36:YQ:21:THR:HB    | 36:YQ:22:LYS:H    | 1.42                     | 0.44              |
| 36:YQ:81:VAL:HG23  | 36:YQ:82:ARG:N    | 2.32                     | 0.44              |
| 40:YU:81:HIS:O     | 40:YU:82:GLY:C    | 2.61                     | 0.44              |
| 42:YW:88:ARG:HH11  | 42:YW:88:ARG:HG2  | 1.82                     | 0.44              |
| 44:YY:88:LYS:HB3   | 44:YY:90:LEU:CD2  | 2.48                     | 0.44              |
| 47:Y1:82:LEU:HD12  | 47:Y1:82:LEU:O    | 2.10                     | 0.44              |
| 1:QA:1347:G:N2     | 1:QA:1373:G:H2'   | 2.33                     | 0.43              |
| 2:QB:87:ARG:HH11   | 2:QB:223:ILE:HD11 | 1.82                     | 0.43              |
| 3:QC:106:VAL:HG11  | 3:QC:109:PRO:HA   | 2.00                     | 0.43              |
| 4:QD:109:GLY:C     | 4:QD:111:ALA:N    | 2.76                     | 0.43              |
| 10:QJ:10:GLY:O     | 10:QJ:68:HIS:N    | 2.51                     | 0.43              |
| 10:QJ:100:THR:O    | 10:QJ:101:VAL:HB  | 2.17                     | 0.43              |
| 11:QK:72:ALA:C     | 11:QK:74:ALA:H    | 2.26                     | 0.43              |
| 12:QL:119:LYS:HB2  | 12:QL:120:TYR:HD1 | 1.83                     | 0.43              |
| 15:QO:25:THR:HG22  | 15:QO:70:LEU:HD22 | 1.99                     | 0.43              |
| 16:QP:68:ASP:C     | 16:QP:70:ALA:N    | 2.75                     | 0.43              |
| 20:QT:50:GLU:O     | 20:QT:52:ALA:N    | 2.51                     | 0.43              |
| 25:RA:271(C):U:H4' | 25:RA:271:G:OP2   | 2.17                     | 0.43              |
| 25:RA:507:A:C5'    | 25:RA:508:G:H5'   | 2.48                     | 0.43              |
| 25:RA:1116:C:H2'   | 25:RA:1117:G:H8   | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:2477:C:H2'  | 55:R9:1:MET:CG    | 2.48                     | 0.43              |
| 25:RA:2729:G:C1'  | 28:RE:187:ALA:HB2 | 2.36                     | 0.43              |
| 27:RD:102:LYS:O   | 27:RD:103:ARG:CG  | 2.66                     | 0.43              |
| 28:RE:3:GLY:CA    | 28:RE:81:ILE:HG21 | 2.48                     | 0.43              |
| 29:RF:24:LEU:HD12 | 29:RF:24:LEU:N    | 2.33                     | 0.43              |
| 36:RQ:27:VAL:HG13 | 36:RQ:28:ALA:N    | 2.32                     | 0.43              |
| 37:RR:75:LEU:C    | 37:RR:75:LEU:CD1  | 2.91                     | 0.43              |
| 39:RT:29:ARG:HA   | 39:RT:45:PHE:O    | 2.17                     | 0.43              |
| 39:RT:99:LEU:CD1  | 39:RT:99:LEU:O    | 2.65                     | 0.43              |
| 39:RT:105:LEU:C   | 39:RT:107:ASP:N   | 2.74                     | 0.43              |
| 41:RV:35:LEU:C    | 41:RV:37:VAL:N    | 2.75                     | 0.43              |
| 42:RW:70:TYR:HD2  | 42:RW:70:TYR:N    | 2.06                     | 0.43              |
| 44:RY:11:ASP:HB2  | 44:RY:27:VAL:CG1  | 2.46                     | 0.43              |
| 44:RY:25:GLY:HA3  | 44:RY:39:VAL:CG1  | 2.47                     | 0.43              |
| 44:RY:48:ALA:CB   | 44:RY:61:ILE:HD13 | 2.45                     | 0.43              |
| 47:R1:80:LEU:O    | 47:R1:81:LYS:CD   | 2.65                     | 0.43              |
| 50:R4:39:CYS:O    | 50:R4:40:HIS:CB   | 2.66                     | 0.43              |
| 50:R4:50:VAL:O    | 50:R4:50:VAL:CG1  | 2.63                     | 0.43              |
| 52:R6:7:ILE:HG23  | 52:R6:8:LYS:N     | 2.32                     | 0.43              |
| 52:R6:11:LEU:HD12 | 52:R6:51:GLU:HG3  | 2.00                     | 0.43              |
| 52:R6:15:GLU:HB3  | 52:R6:16:CYS:H    | 1.46                     | 0.43              |
| 54:R8:58:ILE:O    | 54:R8:61:LEU:CG   | 2.66                     | 0.43              |
| 1:XA:41:G:H2'     | 1:XA:42:G:C8      | 2.54                     | 0.43              |
| 1:XA:599:C:H2'    | 1:XA:600:C:H6     | 1.83                     | 0.43              |
| 1:XA:1000:A:H2'   | 1:XA:1001:G:C8    | 2.53                     | 0.43              |
| 1:XA:1054:C:HO2'  | 1:XA:1055:A:P     | 2.40                     | 0.43              |
| 1:XA:1126:U:H1'   | 1:XA:1280:A:N7    | 2.33                     | 0.43              |
| 1:XA:1388:C:H2'   | 1:XA:1389:C:H6    | 1.83                     | 0.43              |
| 2:XB:95:GLN:HE21  | 2:XB:147:LYS:CE   | 2.28                     | 0.43              |
| 3:XC:59:ARG:HH12  | 3:XC:97:LYS:CD    | 2.31                     | 0.43              |
| 5:XE:31:LEU:HD23  | 5:XE:45:PHE:CD1   | 2.53                     | 0.43              |
| 5:XE:80:ILE:C     | 5:XE:81:GLU:HG2   | 2.43                     | 0.43              |
| 5:XE:154:GLY:O    | 5:XE:155:GLU:C    | 2.62                     | 0.43              |
| 6:XF:72:VAL:HG23  | 6:XF:90:VAL:HG11  | 1.98                     | 0.43              |
| 7:XG:23:VAL:C     | 7:XG:27:ILE:HD13  | 2.43                     | 0.43              |
| 9:XI:29:ASN:OD1   | 9:XI:65:VAL:N     | 2.48                     | 0.43              |
| 10:XJ:96:ILE:N    | 10:XJ:96:ILE:CD1  | 2.79                     | 0.43              |
| 10:XJ:96:ILE:HD13 | 10:XJ:96:ILE:H    | 1.83                     | 0.43              |
| 12:XL:6:THR:H     | 12:XL:9:GLN:NE2   | 1.97                     | 0.43              |
| 13:XM:39:ILE:HD12 | 13:XM:56:LEU:HD23 | 1.99                     | 0.43              |
| 16:XP:20:VAL:HG22 | 16:XP:21:VAL:H    | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:XS:10:PHE:CD1   | 19:XS:38:SER:HB2   | 2.52                     | 0.43              |
| 20:XT:59:ALA:C     | 20:XT:61:SER:N     | 2.75                     | 0.43              |
| 25:YA:704:G:H1'    | 25:YA:727:A:H61    | 1.83                     | 0.43              |
| 25:YA:2286:A:H4'   | 25:YA:2287:A:O4'   | 2.18                     | 0.43              |
| 25:YA:2316:C:H2'   | 25:YA:2317:C:H6    | 1.82                     | 0.43              |
| 25:YA:2682:U:O2'   | 39:YT:58:ASN:ND2   | 2.51                     | 0.43              |
| 27:YD:30:GLU:HG3   | 27:YD:63:ARG:NE    | 2.32                     | 0.43              |
| 27:YD:35:LYS:HB3   | 27:YD:36:PRO:HA    | 2.00                     | 0.43              |
| 27:YD:166:GLN:CA   | 27:YD:166:GLN:NE2  | 2.78                     | 0.43              |
| 28:YE:3:GLY:HA3    | 28:YE:81:ILE:CD1   | 2.47                     | 0.43              |
| 31:YH:137:ASP:OD1  | 31:YH:138:LYS:N    | 2.51                     | 0.43              |
| 34:YO:77:ILE:O     | 34:YO:77:ILE:HG23  | 2.17                     | 0.43              |
| 34:YO:91:LEU:N     | 34:YO:91:LEU:CD2   | 2.80                     | 0.43              |
| 35:YP:70:GLN:N     | 35:YP:70:GLN:OE1   | 2.51                     | 0.43              |
| 41:YV:27:ALA:O     | 41:YV:28:GLU:C     | 2.61                     | 0.43              |
| 41:YV:66:ARG:NH1   | 41:YV:88:ARG:CD    | 2.74                     | 0.43              |
| 50:Y4:48:ARG:NH1   | 50:Y4:51:ASP:HA    | 2.33                     | 0.43              |
| 1:QA:779:C:H4'     | 11:QK:121:PRO:O    | 2.18                     | 0.43              |
| 1:QA:940:C:H2'     | 1:QA:941:G:H8      | 1.83                     | 0.43              |
| 1:QA:1316:G:H22    | 1:QA:1319:A:H5'    | 1.82                     | 0.43              |
| 2:QB:115:LEU:HD21  | 2:QB:153:ARG:HD3   | 1.99                     | 0.43              |
| 2:QB:204:ASN:ND2   | 2:QB:204:ASN:C     | 2.76                     | 0.43              |
| 4:QD:90:GLY:HA3    | 4:QD:204:ILE:HD11  | 2.00                     | 0.43              |
| 9:QI:43:ALA:O      | 9:QI:45:ALA:N      | 2.51                     | 0.43              |
| 10:QJ:6:ILE:O      | 10:QJ:71:LEU:HD12  | 2.18                     | 0.43              |
| 10:QJ:8:LEU:C      | 10:QJ:16:LEU:HD21  | 2.44                     | 0.43              |
| 16:QP:23:ASP:O     | 16:QP:26:ARG:HB2   | 2.18                     | 0.43              |
| 19:QS:51:VAL:HG12  | 19:QS:52:TYR:N     | 2.33                     | 0.43              |
| 25:RA:1313:U:H2'   | 25:RA:1610:A:C2    | 2.53                     | 0.43              |
| 25:RA:1422:G:C6    | 25:RA:1423:G:C5    | 3.06                     | 0.43              |
| 25:RA:1871:A:H2'   | 25:RA:1872:A:C8    | 2.53                     | 0.43              |
| 26:RB:34:U:O4      | 26:RB:44:G:H2'     | 2.17                     | 0.43              |
| 26:RB:44:G:O2'     | 26:RB:48:A:N6      | 2.51                     | 0.43              |
| 27:RD:227:ASN:CB   | 27:RD:228:PRO:CD   | 2.93                     | 0.43              |
| 28:RE:31:CYS:HB3   | 28:RE:49:LEU:HG    | 2.01                     | 0.43              |
| 28:RE:51:PHE:CD1   | 28:RE:52:LEU:N     | 2.76                     | 0.43              |
| 29:RF:167:ALA:HB1  | 29:RF:173:VAL:HG11 | 1.99                     | 0.43              |
| 31:RH:136:ILE:HD12 | 31:RH:136:ILE:N    | 2.31                     | 0.43              |
| 33:RN:30:ILE:HG22  | 33:RN:34:LEU:CD2   | 2.48                     | 0.43              |
| 33:RN:112:LEU:C    | 33:RN:114:ARG:O    | 2.61                     | 0.43              |
| 34:RO:97:ARG:HA    | 34:RO:117:LEU:HD22 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:RP:75:ILE:HG12 | 35:RP:77:ARG:NH1   | 2.32                     | 0.43              |
| 41:RV:66:ARG:NH1  | 41:RV:88:ARG:CD    | 2.74                     | 0.43              |
| 43:RX:7:VAL:O     | 43:RX:30:VAL:CG1   | 2.67                     | 0.43              |
| 43:RX:31:HIS:HA   | 43:RX:32:PRO:HD3   | 1.88                     | 0.43              |
| 44:RY:95:LYS:HA   | 44:RY:101:LYS:N    | 2.33                     | 0.43              |
| 46:R0:41:ARG:HA   | 46:R0:41:ARG:HE    | 1.82                     | 0.43              |
| 52:R6:20:ASN:O    | 52:R6:21:TYR:CG    | 2.71                     | 0.43              |
| 1:XA:390:C:H2'    | 1:XA:391:G:C8      | 2.53                     | 0.43              |
| 1:XA:701:C:H1'    | 1:XA:703:G:C2      | 2.52                     | 0.43              |
| 1:XA:881:G:OP2    | 12:XL:12:ARG:NH2   | 2.51                     | 0.43              |
| 1:XA:973:G:O6     | 1:XA:974:A:N6      | 2.51                     | 0.43              |
| 1:XA:1299:A:H2'   | 1:XA:1301:U:H1'    | 1.99                     | 0.43              |
| 1:XA:1364:U:HO2'  | 1:XA:1365:G:P      | 2.41                     | 0.43              |
| 2:XB:77:ALA:HB1   | 2:XB:165:VAL:HG11  | 2.01                     | 0.43              |
| 7:XG:78:ARG:HH11  | 7:XG:78:ARG:CG     | 2.30                     | 0.43              |
| 7:XG:96:GLN:O     | 7:XG:97:GLN:C      | 2.61                     | 0.43              |
| 8:XH:45:ILE:C     | 8:XH:47:GLY:N      | 2.76                     | 0.43              |
| 13:XM:57:ARG:HH21 | 50:Y4:34:GLU:HA    | 1.83                     | 0.43              |
| 14:XN:17:LYS:HG3  | 14:XN:18:VAL:N     | 2.33                     | 0.43              |
| 14:XN:51:GLY:C    | 14:XN:53:LEU:H     | 2.27                     | 0.43              |
| 18:XR:20:ALA:O    | 18:XR:21:LYS:HG3   | 2.18                     | 0.43              |
| 18:XR:82:THR:CG2  | 18:XR:83:GLU:N     | 2.79                     | 0.43              |
| 20:XT:36:LEU:HD13 | 20:XT:36:LEU:HA    | 1.82                     | 0.43              |
| 22:XV:49:G:O6     | 22:XV:65:C:N4      | 2.49                     | 0.43              |
| 25:YA:340:A:H2'   | 25:YA:341:G:O4'    | 2.19                     | 0.43              |
| 25:YA:554:U:H2'   | 25:YA:556:G:C8     | 2.53                     | 0.43              |
| 25:YA:922:U:H2'   | 25:YA:923:C:C6     | 2.53                     | 0.43              |
| 25:YA:960:A:H5''  | 25:YA:961:C:OP1    | 2.18                     | 0.43              |
| 25:YA:2414:G:H21  | 35:YP:67:MET:CE    | 2.31                     | 0.43              |
| 25:YA:2468:G:O2'  | 25:YA:2481:G:N2    | 2.50                     | 0.43              |
| 32:YI:79:ILE:HB   | 32:YI:142:VAL:HA   | 2.00                     | 0.43              |
| 32:YI:130:TYR:HB3 | 32:YI:136:VAL:HG13 | 1.99                     | 0.43              |
| 35:YP:19:VAL:HG22 | 35:YP:21:ARG:H     | 1.83                     | 0.43              |
| 35:YP:101:VAL:HA  | 35:YP:106:LEU:HB2  | 1.99                     | 0.43              |
| 37:YR:33:ARG:HA   | 37:YR:114:VAL:O    | 2.18                     | 0.43              |
| 37:YR:74:LYS:O    | 37:YR:76:VAL:N     | 2.45                     | 0.43              |
| 38:YS:14:VAL:CG1  | 38:YS:15:ARG:N     | 2.81                     | 0.43              |
| 38:YS:38:GLN:CG   | 38:YS:47:THR:HG21  | 2.48                     | 0.43              |
| 38:YS:57:LYS:O    | 38:YS:58:LEU:HB3   | 2.18                     | 0.43              |
| 38:YS:86:ALA:O    | 38:YS:87:PHE:CB    | 2.65                     | 0.43              |
| 38:YS:99:LYS:C    | 38:YS:101:LEU:H    | 2.25                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:107:ASP:OD2  | 39:YT:109:GLU:HB2  | 2.19                     | 0.43              |
| 41:YV:66:ARG:NH1   | 41:YV:88:ARG:NH1   | 2.61                     | 0.43              |
| 42:YW:29:LEU:HD11  | 42:YW:55:ALA:HB2   | 1.98                     | 0.43              |
| 43:YX:3:THR:HA     | 43:YX:6:ASP:OD2    | 2.18                     | 0.43              |
| 47:Y1:94:LEU:O     | 47:Y1:95:LEU:HB2   | 2.17                     | 0.43              |
| 1:QA:109:A:H2'     | 1:QA:326:G:H21     | 1.82                     | 0.43              |
| 1:QA:299:G:H2'     | 1:QA:300:A:C8      | 2.53                     | 0.43              |
| 1:QA:555:C:H2'     | 1:QA:556:C:C6      | 2.53                     | 0.43              |
| 1:QA:769:G:H4'     | 1:QA:1513:A:H4'    | 2.00                     | 0.43              |
| 2:QB:37:ASN:C      | 2:QB:39:ILE:N      | 2.73                     | 0.43              |
| 2:QB:100:GLY:N     | 2:QB:176:GLU:OE2   | 2.51                     | 0.43              |
| 4:QD:71:SER:O      | 4:QD:72:GLU:C      | 2.60                     | 0.43              |
| 7:QG:15:ASP:OD1    | 7:QG:23:VAL:HG11   | 2.19                     | 0.43              |
| 7:QG:23:VAL:C      | 7:QG:27:ILE:HD13   | 2.44                     | 0.43              |
| 7:QG:38:LEU:O      | 7:QG:42:ILE:HG13   | 2.17                     | 0.43              |
| 10:QJ:90:LEU:N     | 10:QJ:91:PRO:CD    | 2.81                     | 0.43              |
| 11:QK:75:TYR:N     | 11:QK:75:TYR:CD1   | 2.85                     | 0.43              |
| 12:QL:44:THR:HA    | 12:QL:45:PRO:HD3   | 1.71                     | 0.43              |
| 13:QM:19:LEU:HD22  | 13:QM:19:LEU:N     | 2.33                     | 0.43              |
| 14:QN:51:GLY:C     | 14:QN:53:LEU:H     | 2.27                     | 0.43              |
| 19:QS:45:VAL:O     | 19:QS:62:ILE:O     | 2.36                     | 0.43              |
| 25:RA:134:C:H2'    | 25:RA:135:G:H8     | 1.84                     | 0.43              |
| 25:RA:512:G:O2'    | 25:RA:513:A:P      | 2.76                     | 0.43              |
| 25:RA:750:A:OP1    | 25:RA:1615:C:N4    | 2.50                     | 0.43              |
| 25:RA:1278:A:OP1   | 37:RR:36:THR:HG22  | 2.18                     | 0.43              |
| 25:RA:1394:U:C4    | 25:RA:1395:A:C6    | 3.06                     | 0.43              |
| 25:RA:1598:C:H2'   | 25:RA:1599:C:H6    | 1.82                     | 0.43              |
| 25:RA:2593:U:H2'   | 25:RA:2594:C:C6    | 2.52                     | 0.43              |
| 25:RA:2659:G:N2    | 25:RA:2662:A:OP2   | 2.52                     | 0.43              |
| 28:RE:16:ARG:O     | 28:RE:18:ASP:O     | 2.36                     | 0.43              |
| 28:RE:36:ARG:HB3   | 28:RE:36:ARG:NH1   | 2.30                     | 0.43              |
| 29:RF:101:LEU:HD12 | 29:RF:102:PRO:N    | 2.33                     | 0.43              |
| 29:RF:149:ASP:OD2  | 29:RF:151:SER:HB3  | 2.17                     | 0.43              |
| 30:RG:19:LEU:HA    | 30:RG:22:ARG:HB2   | 1.99                     | 0.43              |
| 30:RG:139:LEU:HA   | 30:RG:144:ILE:HG21 | 2.00                     | 0.43              |
| 31:RH:137:ASP:OD1  | 31:RH:138:LYS:N    | 2.51                     | 0.43              |
| 33:RN:99:LEU:O     | 33:RN:100:GLU:C    | 2.60                     | 0.43              |
| 35:RP:81:GLN:HE21  | 35:RP:81:GLN:HB2   | 1.59                     | 0.43              |
| 35:RP:101:VAL:HG13 | 35:RP:102:ARG:N    | 2.33                     | 0.43              |
| 37:RR:81:ASP:N     | 37:RR:81:ASP:OD2   | 2.50                     | 0.43              |
| 41:RV:15:GLU:O     | 41:RV:96:ILE:HB    | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:RV:25:LEU:H     | 41:RV:92:THR:CG2   | 2.28                     | 0.43              |
| 47:R1:53:VAL:CG1   | 47:R1:54:ALA:N     | 2.81                     | 0.43              |
| 53:R7:5:TRP:CD1    | 53:R7:7:PRO:HG3    | 2.53                     | 0.43              |
| 54:R8:58:ILE:O     | 54:R8:61:LEU:CD1   | 2.67                     | 0.43              |
| 1:XA:34:C:H2'      | 1:XA:35:G:H8       | 1.83                     | 0.43              |
| 1:XA:452:A:H2'     | 1:XA:453:A:C8      | 2.54                     | 0.43              |
| 1:XA:1312:G:H3'    | 50:Y4:67:TYR:OH    | 2.18                     | 0.43              |
| 1:XA:1312:G:N7     | 19:XS:2:PRO:HD2    | 2.34                     | 0.43              |
| 2:XB:47:THR:HG22   | 2:XB:51:LEU:CG     | 2.48                     | 0.43              |
| 2:XB:162:ILE:O     | 2:XB:185:ILE:HG13  | 2.18                     | 0.43              |
| 3:XC:6:HIS:C       | 3:XC:8:ILE:N       | 2.76                     | 0.43              |
| 3:XC:27:LYS:HB3    | 3:XC:27:LYS:NZ     | 2.34                     | 0.43              |
| 4:XD:95:GLY:O      | 4:XD:99:SER:N      | 2.51                     | 0.43              |
| 5:XE:67:VAL:HG22   | 5:XE:68:GLU:N      | 2.33                     | 0.43              |
| 6:XF:48:LEU:HD23   | 6:XF:48:LEU:HA     | 1.85                     | 0.43              |
| 6:XF:91:VAL:CG1    | 18:XR:72:ARG:NH1   | 2.82                     | 0.43              |
| 11:XK:108:ILE:HG21 | 18:XR:88:LYS:OXT   | 2.19                     | 0.43              |
| 25:YA:99:U:H4'     | 25:YA:101:G:O5'    | 2.19                     | 0.43              |
| 25:YA:2219:G:H5''  | 27:YD:269:PHE:CZ   | 2.52                     | 0.43              |
| 25:YA:2732:G:H3'   | 25:YA:2733:A:O4'   | 2.19                     | 0.43              |
| 27:YD:43:ARG:CZ    | 27:YD:49:ILE:HG21  | 2.49                     | 0.43              |
| 29:YF:79:GLY:O     | 29:YF:80:ALA:C     | 2.61                     | 0.43              |
| 30:YG:136:ARG:O    | 30:YG:154:GLY:CA   | 2.62                     | 0.43              |
| 31:YH:136:ILE:HD12 | 31:YH:136:ILE:N    | 2.31                     | 0.43              |
| 32:YI:93:THR:O     | 32:YI:97:ILE:HG12  | 2.18                     | 0.43              |
| 34:YO:63:VAL:O     | 34:YO:63:VAL:HG23  | 2.17                     | 0.43              |
| 37:YR:75:LEU:C     | 37:YR:75:LEU:CD1   | 2.91                     | 0.43              |
| 39:YT:29:ARG:HA    | 39:YT:45:PHE:O     | 2.17                     | 0.43              |
| 39:YT:49:VAL:O     | 39:YT:49:VAL:CG1   | 2.64                     | 0.43              |
| 39:YT:114:LEU:HA   | 39:YT:114:LEU:HD23 | 1.74                     | 0.43              |
| 39:YT:118:ARG:O    | 39:YT:119:LYS:C    | 2.60                     | 0.43              |
| 40:YU:90:VAL:C     | 40:YU:92:ARG:N     | 2.77                     | 0.43              |
| 42:YW:50:VAL:O     | 42:YW:53:SER:N     | 2.50                     | 0.43              |
| 42:YW:67:ASP:OD2   | 42:YW:67:ASP:N     | 2.50                     | 0.43              |
| 44:YY:95:LYS:HB2   | 44:YY:99:CYS:O     | 2.17                     | 0.43              |
| 45:YZ:54:HIS:CG    | 45:YZ:101:PRO:HG3  | 2.54                     | 0.43              |
| 47:Y1:60:PHE:HZ    | 47:Y1:90:ILE:HG21  | 1.82                     | 0.43              |
| 50:Y4:2:LYS:HD2    | 50:Y4:2:LYS:HA     | 1.61                     | 0.43              |
| 52:Y6:11:LEU:HD12  | 52:Y6:51:GLU:HG3   | 2.00                     | 0.43              |
| 53:Y7:17:GLY:O     | 53:Y7:20:ALA:HB3   | 2.18                     | 0.43              |
| 54:Y8:58:ILE:O     | 54:Y8:61:LEU:CG    | 2.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:Y8:58:ILE:O     | 54:Y8:61:LEU:CD1   | 2.67                     | 0.43              |
| 1:QA:17:U:H2'      | 1:QA:18:C:C6       | 2.53                     | 0.43              |
| 1:QA:474:G:H2'     | 1:QA:475:G:C8      | 2.53                     | 0.43              |
| 1:QA:753:A:H4'     | 1:QA:754:C:O5'     | 2.18                     | 0.43              |
| 1:QA:935:A:H61     | 7:QG:3:ARG:HG3     | 1.84                     | 0.43              |
| 1:QA:986:A:H1'     | 19:QS:54:GLY:O     | 2.18                     | 0.43              |
| 1:QA:1065:U:C5     | 1:QA:1190:G:H1'    | 2.53                     | 0.43              |
| 2:QB:231:GLU:HA    | 2:QB:232:PRO:HD3   | 1.83                     | 0.43              |
| 3:QC:69:HIS:HA     | 3:QC:104:GLN:HB2   | 2.00                     | 0.43              |
| 4:QD:132:ARG:HH11  | 4:QD:132:ARG:HG2   | 1.83                     | 0.43              |
| 6:QF:88:VAL:HG12   | 6:QF:89:MET:N      | 2.34                     | 0.43              |
| 7:QG:23:VAL:O      | 7:QG:27:ILE:HD12   | 2.19                     | 0.43              |
| 7:QG:49:ILE:C      | 7:QG:51:GLN:H      | 2.26                     | 0.43              |
| 7:QG:78:ARG:HH11   | 7:QG:78:ARG:CG     | 2.31                     | 0.43              |
| 9:QI:10:ARG:NE     | 9:QI:105:ASP:CB    | 2.81                     | 0.43              |
| 9:QI:41:VAL:HG12   | 9:QI:41:VAL:O      | 2.18                     | 0.43              |
| 11:QK:105:VAL:O    | 11:QK:105:VAL:HG23 | 2.19                     | 0.43              |
| 13:QM:107:ALA:O    | 13:QM:108:ARG:C    | 2.62                     | 0.43              |
| 16:QP:21:VAL:HG23  | 16:QP:34:GLU:N     | 2.34                     | 0.43              |
| 19:QS:12:ASP:CG    | 19:QS:37:ARG:HD2   | 2.43                     | 0.43              |
| 19:QS:36:ARG:NH1   | 19:QS:52:TYR:O     | 2.51                     | 0.43              |
| 22:QV:15:G:N2      | 22:QV:48:C:H42     | 2.17                     | 0.43              |
| 25:RA:302:C:H2'    | 25:RA:303:U:H6     | 1.83                     | 0.43              |
| 25:RA:662:G:H5''   | 35:RP:15:ARG:O     | 2.18                     | 0.43              |
| 25:RA:1184:G:C6    | 25:RA:1185:C:C4    | 3.06                     | 0.43              |
| 25:RA:2405:G:O2'   | 25:RA:2406:U:P     | 2.76                     | 0.43              |
| 25:RA:2753:A:O2'   | 55:R9:15:LYS:NZ    | 2.52                     | 0.43              |
| 25:RA:2882:A:OP1   | 37:RR:96:ARG:NH1   | 2.52                     | 0.43              |
| 26:RB:28:C:H2'     | 26:RB:29:A:C8      | 2.54                     | 0.43              |
| 26:RB:44:G:H1'     | 26:RB:47:C:H42     | 1.84                     | 0.43              |
| 26:RB:116:G:H4'    | 38:RS:54:LEU:HD13  | 2.00                     | 0.43              |
| 27:RD:69:ARG:NH2   | 27:RD:130:ALA:HB2  | 2.19                     | 0.43              |
| 28:RE:7:VAL:HG11   | 39:RT:1:MET:HE3    | 2.00                     | 0.43              |
| 28:RE:16:ARG:C     | 28:RE:17:ASP:CG    | 2.86                     | 0.43              |
| 28:RE:52:LEU:O     | 28:RE:74:PRO:HA    | 2.18                     | 0.43              |
| 29:RF:63:LYS:CE    | 29:RF:67:GLN:HB2   | 2.49                     | 0.43              |
| 29:RF:201:VAL:HG13 | 29:RF:202:PHE:N    | 2.33                     | 0.43              |
| 30:RG:59:GLU:O     | 30:RG:62:LEU:HB3   | 2.18                     | 0.43              |
| 30:RG:125:PHE:C    | 30:RG:127:GLY:N    | 2.76                     | 0.43              |
| 30:RG:131:TYR:HE2  | 30:RG:133:LEU:HD22 | 1.84                     | 0.43              |
| 31:RH:92:ILE:CD1   | 31:RH:160:LYS:HD3  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:RP:47:ASP:CG   | 35:RP:49:ARG:NH1   | 2.77                     | 0.43              |
| 38:RS:99:LYS:C    | 38:RS:101:LEU:H    | 2.25                     | 0.43              |
| 40:RU:88:ILE:HG22 | 40:RU:90:VAL:CG2   | 2.44                     | 0.43              |
| 50:R4:49:PHE:N    | 50:R4:49:PHE:HD1   | 2.17                     | 0.43              |
| 1:XA:41:G:H2'     | 1:XA:42:G:H8       | 1.83                     | 0.43              |
| 1:XA:390:C:O3'    | 16:XP:28:ARG:NH2   | 2.51                     | 0.43              |
| 1:XA:430:A:OP1    | 4:XD:9:CYS:HB2     | 2.18                     | 0.43              |
| 1:XA:637:G:H2'    | 1:XA:638:G:H8      | 1.83                     | 0.43              |
| 1:XA:1388:C:H2'   | 1:XA:1389:C:C6     | 2.53                     | 0.43              |
| 2:XB:115:LEU:HD21 | 2:XB:153:ARG:HD3   | 2.00                     | 0.43              |
| 2:XB:207:ALA:C    | 2:XB:209:ARG:N     | 2.76                     | 0.43              |
| 3:XC:22:TRP:CB    | 3:XC:59:ARG:HB2    | 2.48                     | 0.43              |
| 4:XD:163:GLU:OE2  | 4:XD:163:GLU:HA    | 2.19                     | 0.43              |
| 7:XG:62:PHE:O     | 7:XG:64:GLN:N      | 2.51                     | 0.43              |
| 7:XG:148:ASN:O    | 7:XG:150:ALA:N     | 2.51                     | 0.43              |
| 8:XH:21:LYS:O     | 8:XH:65:TYR:OH     | 2.36                     | 0.43              |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:H     | 1.84                     | 0.43              |
| 13:XM:87:TYR:HA   | 13:XM:90:LEU:HG    | 2.01                     | 0.43              |
| 13:XM:107:ALA:O   | 13:XM:108:ARG:C    | 2.61                     | 0.43              |
| 18:XR:67:ALA:O    | 18:XR:68:LYS:C     | 2.62                     | 0.43              |
| 19:XS:5:LEU:CG    | 50:Y4:66:SER:HB2   | 2.47                     | 0.43              |
| 25:YA:902:C:H2'   | 25:YA:903:C:C6     | 2.53                     | 0.43              |
| 25:YA:1105:U:H2'  | 25:YA:1106:G:H8    | 1.83                     | 0.43              |
| 25:YA:1783:A:H5'  | 25:YA:2608:G:H4'   | 2.01                     | 0.43              |
| 28:YE:11:MET:O    | 28:YE:12:THR:HB    | 2.18                     | 0.43              |
| 31:YH:92:ILE:CD1  | 31:YH:160:LYS:HD3  | 2.48                     | 0.43              |
| 31:YH:149:ARG:HA  | 31:YH:162:ILE:HG21 | 1.99                     | 0.43              |
| 32:YI:13:GLY:HA3  | 32:YI:17:GLN:OE1   | 2.19                     | 0.43              |
| 33:YN:17:ASP:O    | 33:YN:55:VAL:O     | 2.34                     | 0.43              |
| 33:YN:133:GLN:C   | 33:YN:134:ARG:HG2  | 2.41                     | 0.43              |
| 35:YP:96:THR:HG22 | 35:YP:126:VAL:CB   | 2.47                     | 0.43              |
| 42:YW:111:HIS:CG  | 42:YW:112:GLY:H    | 2.37                     | 0.43              |
| 43:YX:14:SER:HB2  | 43:YX:15:GLU:OE1   | 2.19                     | 0.43              |
| 43:YX:70:LEU:HD23 | 43:YX:70:LEU:H     | 1.78                     | 0.43              |
| 45:YZ:182:LYS:CG  | 45:YZ:183:LEU:HA   | 2.47                     | 0.43              |
| 48:Y2:59:ARG:O    | 48:Y2:62:THR:HG23  | 2.18                     | 0.43              |
| 50:Y4:59:PHE:CE1  | 50:Y4:70:GLY:N     | 2.87                     | 0.43              |
| 52:Y6:20:ASN:O    | 52:Y6:21:TYR:CG    | 2.71                     | 0.43              |
| 53:Y7:19:ARG:HG2  | 53:Y7:19:ARG:NH1   | 2.34                     | 0.43              |
| 54:Y8:40:GLU:O    | 54:Y8:43:GLN:N     | 2.50                     | 0.43              |
| 55:Y9:1:MET:HE1   | 55:Y9:32:HIS:CD2   | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:21:G:H2'      | 1:QA:22:G:C8       | 2.54                     | 0.43              |
| 1:QA:1320:C:N4     | 19:QS:36:ARG:HG3   | 2.34                     | 0.43              |
| 1:QA:1372:U:OP1    | 9:QI:71:SER:HB3    | 2.18                     | 0.43              |
| 2:QB:32:ILE:HD13   | 2:QB:190:THR:CG2   | 2.48                     | 0.43              |
| 2:QB:47:THR:O      | 2:QB:51:LEU:N      | 2.32                     | 0.43              |
| 2:QB:142:LEU:HD23  | 2:QB:142:LEU:O     | 2.19                     | 0.43              |
| 4:QD:95:GLY:O      | 4:QD:99:SER:N      | 2.51                     | 0.43              |
| 6:QF:91:VAL:CG1    | 18:QR:72:ARG:NH1   | 2.82                     | 0.43              |
| 7:QG:88:PRO:HB3    | 7:QG:145:ALA:HA    | 2.01                     | 0.43              |
| 8:QH:45:ILE:C      | 8:QH:47:GLY:N      | 2.76                     | 0.43              |
| 10:QJ:51:ARG:HG2   | 10:QJ:51:ARG:NH1   | 2.33                     | 0.43              |
| 10:QJ:54:PHE:CE2   | 10:QJ:55:LYS:HD2   | 2.52                     | 0.43              |
| 11:QK:62:GLN:O     | 11:QK:64:ALA:N     | 2.52                     | 0.43              |
| 15:QO:77:ARG:HA    | 15:QO:80:ALA:HB2   | 1.99                     | 0.43              |
| 16:QP:72:ARG:HD3   | 16:QP:72:ARG:O     | 2.17                     | 0.43              |
| 25:RA:137(A):G:H2' | 25:RA:139:G:N7     | 2.32                     | 0.43              |
| 25:RA:954:G:O2'    | 25:RA:2274:A:N1    | 2.41                     | 0.43              |
| 25:RA:1139:G:P     | 33:RN:101:HIS:CE1  | 3.12                     | 0.43              |
| 25:RA:2250:G:C4    | 36:RQ:82:ARG:HG3   | 2.54                     | 0.43              |
| 25:RA:2322:A:H2'   | 25:RA:2323:G:O4'   | 2.19                     | 0.43              |
| 26:RB:104:A:H2'    | 26:RB:105:G:O4'    | 2.18                     | 0.43              |
| 27:RD:17:THR:HG22  | 27:RD:204:ILE:HA   | 1.98                     | 0.43              |
| 29:RF:198:ALA:C    | 29:RF:200:GLU:H    | 2.25                     | 0.43              |
| 32:RI:93:THR:HG22  | 32:RI:119:PRO:HB3  | 2.00                     | 0.43              |
| 35:RP:12:ALA:C     | 35:RP:14:LYS:N     | 2.73                     | 0.43              |
| 35:RP:70:GLN:N     | 35:RP:70:GLN:OE1   | 2.51                     | 0.43              |
| 35:RP:107:LYS:HB2  | 35:RP:110:TYR:HD2  | 1.83                     | 0.43              |
| 36:RQ:108:GLY:HA3  | 45:RZ:116:VAL:HG11 | 1.99                     | 0.43              |
| 38:RS:14:VAL:CG1   | 38:RS:15:ARG:N     | 2.81                     | 0.43              |
| 38:RS:56:LEU:O     | 38:RS:57:LYS:O     | 2.36                     | 0.43              |
| 38:RS:57:LYS:O     | 38:RS:58:LEU:HB3   | 2.18                     | 0.43              |
| 38:RS:110:LEU:HD23 | 38:RS:112:PHE:CE2  | 2.53                     | 0.43              |
| 39:RT:89:VAL:O     | 39:RT:90:GLN:HB2   | 2.19                     | 0.43              |
| 40:RU:64:ARG:CG    | 40:RU:64:ARG:NH2   | 2.70                     | 0.43              |
| 40:RU:95:LEU:HD13  | 41:RV:4:ILE:HD12   | 1.98                     | 0.43              |
| 44:RY:6:HIS:ND1    | 44:RY:6:HIS:N      | 2.66                     | 0.43              |
| 45:RZ:52:SER:O     | 45:RZ:52:SER:OG    | 2.31                     | 0.43              |
| 50:R4:68:ARG:O     | 50:R4:69:LYS:HB2   | 2.17                     | 0.43              |
| 1:XA:176:C:O2'     | 1:XA:1451:A:N1     | 2.52                     | 0.43              |
| 1:XA:186:C:H5'     | 20:XT:78:ALA:HB1   | 2.01                     | 0.43              |
| 1:XA:502:G:C2      | 1:XA:503:C:C2      | 3.07                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:752:G:O2'     | 1:XA:753:A:O5'     | 2.32                     | 0.43              |
| 1:XA:1065:U:O2'    | 1:XA:1066:C:OP2    | 2.28                     | 0.43              |
| 2:XB:163:PHE:HD2   | 2:XB:163:PHE:HA    | 1.69                     | 0.43              |
| 2:XB:204:ASN:ND2   | 2:XB:204:ASN:C     | 2.76                     | 0.43              |
| 3:XC:106:VAL:HG11  | 3:XC:109:PRO:HA    | 2.01                     | 0.43              |
| 4:XD:128:VAL:C     | 4:XD:130:GLY:N     | 2.76                     | 0.43              |
| 6:XF:76:ALA:HB1    | 6:XF:80:ARG:HH21   | 1.82                     | 0.43              |
| 9:XI:71:SER:C      | 9:XI:73:GLN:N      | 2.74                     | 0.43              |
| 11:XK:124:LYS:HB3  | 11:XK:125:PHE:H    | 1.68                     | 0.43              |
| 15:XO:25:THR:O     | 15:XO:29:VAL:HG23  | 2.18                     | 0.43              |
| 22:XV:54:U:C4      | 22:XV:55:U:C4      | 3.06                     | 0.43              |
| 25:YA:27:G:H1'     | 25:YA:513:A:H62    | 1.84                     | 0.43              |
| 25:YA:312:G:H5'    | 25:YA:331:A:O2'    | 2.18                     | 0.43              |
| 25:YA:1683:C:H2'   | 25:YA:1684:C:H6    | 1.82                     | 0.43              |
| 27:YD:44:ASN:HB3   | 27:YD:49:ILE:CG2   | 2.47                     | 0.43              |
| 28:YE:13:ARG:HH11  | 28:YE:13:ARG:HB2   | 1.81                     | 0.43              |
| 28:YE:143:ASN:N    | 28:YE:143:ASN:ND2  | 2.65                     | 0.43              |
| 30:YG:44:GLY:HA2   | 30:YG:88:ILE:HD11  | 2.00                     | 0.43              |
| 30:YG:67:LYS:N     | 30:YG:67:LYS:HD2   | 2.33                     | 0.43              |
| 30:YG:114:ILE:O    | 30:YG:116:ASP:N    | 2.51                     | 0.43              |
| 30:YG:131:TYR:HE2  | 30:YG:133:LEU:HD22 | 1.83                     | 0.43              |
| 31:YH:35:VAL:CG2   | 31:YH:75:ALA:HB2   | 2.49                     | 0.43              |
| 34:YO:51:ALA:O     | 34:YO:53:LYS:HE3   | 2.18                     | 0.43              |
| 38:YS:88:ASP:CG    | 38:YS:89:ARG:N     | 2.77                     | 0.43              |
| 38:YS:110:LEU:HD23 | 38:YS:112:PHE:CE2  | 2.54                     | 0.43              |
| 41:YV:35:LEU:HD22  | 41:YV:35:LEU:N     | 2.23                     | 0.43              |
| 42:YW:17:VAL:C     | 42:YW:19:LEU:N     | 2.76                     | 0.43              |
| 44:YY:84:ARG:HD3   | 44:YY:86:ARG:HH11  | 1.83                     | 0.43              |
| 49:Y3:39:ASP:O     | 49:Y3:39:ASP:CG    | 2.62                     | 0.43              |
| 50:Y4:15:ILE:N     | 50:Y4:15:ILE:CD1   | 2.77                     | 0.43              |
| 50:Y4:26:SER:C     | 50:Y4:27:THR:O     | 2.58                     | 0.43              |
| 50:Y4:43:TYR:O     | 50:Y4:46:GLN:HA    | 2.19                     | 0.43              |
| 51:Y5:15:ARG:HA    | 51:Y5:18:ALA:HB3   | 1.99                     | 0.43              |
| 51:Y5:40:LYS:HZ1   | 51:Y5:48:GLU:CB    | 2.20                     | 0.43              |
| 1:QA:35:G:C6       | 1:QA:36:C:N4       | 2.86                     | 0.43              |
| 1:QA:474:G:H5''    | 16:QP:81:ARG:HE    | 1.84                     | 0.43              |
| 1:QA:1001:G:H2'    | 1:QA:1002:G:O4'    | 2.19                     | 0.43              |
| 1:QA:1124:G:H5''   | 1:QA:1145:C:H41    | 1.83                     | 0.43              |
| 1:QA:1277:C:O2'    | 1:QA:1279:A:H8     | 2.02                     | 0.43              |
| 1:QA:1314:C:H5''   | 19:QS:6:LYS:HZ1    | 1.83                     | 0.43              |
| 2:QB:90:MET:HA     | 2:QB:91:PRO:HD3    | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:QB:128:GLU:O    | 2:QB:129:GLU:C    | 2.61                     | 0.43              |
| 3:QC:67:THR:O     | 3:QC:69:HIS:CE1   | 2.72                     | 0.43              |
| 4:QD:163:GLU:OE2  | 4:QD:163:GLU:HA   | 2.19                     | 0.43              |
| 5:QE:62:ALA:O     | 5:QE:64:ARG:N     | 2.51                     | 0.43              |
| 6:QF:61:LEU:HD23  | 6:QF:63:TYR:OH    | 2.17                     | 0.43              |
| 7:QG:111:ARG:HH11 | 7:QG:111:ARG:CB   | 2.23                     | 0.43              |
| 8:QH:21:LYS:O     | 8:QH:65:TYR:OH    | 2.36                     | 0.43              |
| 12:QL:27:LEU:HD13 | 12:QL:28:LYS:H    | 1.84                     | 0.43              |
| 18:QR:43:PHE:HA   | 18:QR:51:LEU:HD12 | 2.01                     | 0.43              |
| 19:QS:21:GLU:HG3  | 19:QS:22:LEU:CD1  | 2.49                     | 0.43              |
| 22:QV:54:U:C4     | 22:QV:55:U:C4     | 3.06                     | 0.43              |
| 25:RA:288:C:H2'   | 25:RA:289:A:C8    | 2.52                     | 0.43              |
| 25:RA:448:U:O4    | 25:RA:583:G:H1'   | 2.19                     | 0.43              |
| 25:RA:646:A:H2'   | 25:RA:647:G:O4'   | 2.18                     | 0.43              |
| 25:RA:822:U:H2'   | 25:RA:823:G:C8    | 2.53                     | 0.43              |
| 25:RA:1041:C:H2'  | 25:RA:1042:G:C8   | 2.53                     | 0.43              |
| 25:RA:1772:G:N2   | 25:RA:1774:C:H5'  | 2.34                     | 0.43              |
| 25:RA:1882:C:H5'  | 25:RA:1883:G:OP2  | 2.19                     | 0.43              |
| 25:RA:2587:A:H8   | 25:RA:2587:A:O5'  | 2.01                     | 0.43              |
| 25:RA:2839:G:H5'  | 37:RR:46:GLY:CA   | 2.49                     | 0.43              |
| 27:RD:177:LEU:O   | 27:RD:179:SER:N   | 2.51                     | 0.43              |
| 28:RE:51:PHE:O    | 28:RE:74:PRO:CB   | 2.67                     | 0.43              |
| 28:RE:120:TRP:CE3 | 28:RE:155:LYS:HD3 | 2.53                     | 0.43              |
| 29:RF:62:ARG:NH1  | 29:RF:62:ARG:CB   | 2.82                     | 0.43              |
| 29:RF:144:LYS:C   | 29:RF:146:ALA:N   | 2.75                     | 0.43              |
| 31:RH:35:VAL:CG2  | 31:RH:75:ALA:HB2  | 2.48                     | 0.43              |
| 34:RO:51:ALA:O    | 34:RO:53:LYS:HE3  | 2.19                     | 0.43              |
| 34:RO:116:SER:C   | 34:RO:118:ALA:N   | 2.76                     | 0.43              |
| 37:RR:54:LEU:O    | 37:RR:62:ALA:HB1  | 2.19                     | 0.43              |
| 37:RR:85:PRO:C    | 37:RR:87:TYR:N    | 2.73                     | 0.43              |
| 39:RT:6:LEU:HD12  | 39:RT:9:LEU:HD12  | 2.00                     | 0.43              |
| 39:RT:105:LEU:O   | 39:RT:105:LEU:HG  | 2.19                     | 0.43              |
| 42:RW:31:GLU:O    | 42:RW:32:ALA:C    | 2.60                     | 0.43              |
| 55:R9:7:VAL:HG21  | 55:R9:36:GLN:HB2  | 2.00                     | 0.43              |
| 1:XA:267:C:OP2    | 17:XQ:67:LYS:HD2  | 2.19                     | 0.43              |
| 1:XA:564:C:H5'    | 17:XQ:32:TYR:CE2  | 2.54                     | 0.43              |
| 1:XA:1502:A:H2'   | 1:XA:1504:G:C8    | 2.54                     | 0.43              |
| 2:XB:132:LYS:HA   | 2:XB:135:GLN:CB   | 2.43                     | 0.43              |
| 4:XD:71:SER:O     | 4:XD:72:GLU:C     | 2.60                     | 0.43              |
| 4:XD:122:ARG:HA   | 4:XD:134:ASP:HB2  | 1.99                     | 0.43              |
| 6:XF:73:ASN:O     | 6:XF:76:ALA:HB3   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:XG:49:ILE:C     | 7:XG:51:GLN:H      | 2.26                     | 0.43              |
| 7:XG:88:PRO:HB3   | 7:XG:145:ALA:HA    | 2.01                     | 0.43              |
| 12:XL:76:ASN:O    | 12:XL:76:ASN:CG    | 2.62                     | 0.43              |
| 15:XO:83:GLU:HA   | 15:XO:83:GLU:OE1   | 2.19                     | 0.43              |
| 18:XR:63:GLN:O    | 18:XR:66:LEU:HB3   | 2.19                     | 0.43              |
| 19:XS:36:ARG:NH1  | 19:XS:52:TYR:O     | 2.51                     | 0.43              |
| 20:XT:50:GLU:O    | 20:XT:52:ALA:N     | 2.51                     | 0.43              |
| 25:YA:1021:A:H8   | 25:YA:1022:G:H5''  | 1.84                     | 0.43              |
| 25:YA:1672:C:H4'  | 25:YA:2553:G:H5''  | 2.01                     | 0.43              |
| 25:YA:2021:C:OP1  | 51:Y5:12:SER:OG    | 2.32                     | 0.43              |
| 25:YA:2846:G:P    | 39:YT:54:ARG:HB2   | 2.58                     | 0.43              |
| 26:YB:9:G:C6      | 26:YB:10:C:C4      | 3.07                     | 0.43              |
| 27:YD:11:PRO:O    | 27:YD:12:SER:OG    | 2.29                     | 0.43              |
| 28:YE:3:GLY:CA    | 28:YE:81:ILE:HG21  | 2.49                     | 0.43              |
| 28:YE:16:ARG:O    | 28:YE:18:ASP:O     | 2.36                     | 0.43              |
| 28:YE:25:VAL:HG21 | 39:YT:8:LYS:HG3    | 2.00                     | 0.43              |
| 28:YE:51:PHE:O    | 28:YE:74:PRO:CB    | 2.67                     | 0.43              |
| 30:YG:145:THR:O   | 30:YG:146:TYR:HB3  | 2.19                     | 0.43              |
| 33:YN:26:LEU:HG   | 33:YN:30:ILE:CD1   | 2.49                     | 0.43              |
| 33:YN:30:ILE:HG22 | 33:YN:34:LEU:CD2   | 2.48                     | 0.43              |
| 36:YQ:25:ASP:H    | 36:YQ:102:VAL:HG23 | 1.84                     | 0.43              |
| 36:YQ:80:GLU:C    | 36:YQ:81:VAL:CG1   | 2.89                     | 0.43              |
| 37:YR:54:LEU:O    | 37:YR:62:ALA:HB1   | 2.19                     | 0.43              |
| 38:YS:30:ARG:NH2  | 38:YS:92:TYR:HD1   | 2.17                     | 0.43              |
| 39:YT:89:VAL:O    | 39:YT:90:GLN:HB2   | 2.19                     | 0.43              |
| 44:YY:6:HIS:ND1   | 44:YY:6:HIS:N      | 2.66                     | 0.43              |
| 44:YY:75:ILE:HG12 | 44:YY:76:CYS:H     | 1.79                     | 0.43              |
| 1:QA:276:G:O3'    | 17:QQ:68:ARG:NH1   | 2.51                     | 0.43              |
| 1:QA:1059:C:H2'   | 1:QA:1060:C:C6     | 2.53                     | 0.43              |
| 2:QB:68:ILE:HB    | 2:QB:70:PHE:HE1    | 1.82                     | 0.43              |
| 2:QB:200:ILE:HD12 | 2:QB:200:ILE:N     | 2.34                     | 0.43              |
| 3:QC:27:LYS:NZ    | 3:QC:27:LYS:HB3    | 2.34                     | 0.43              |
| 3:QC:59:ARG:HH12  | 3:QC:97:LYS:CD     | 2.31                     | 0.43              |
| 5:QE:94:ALA:HB2   | 5:QE:119:LEU:HG    | 2.00                     | 0.43              |
| 6:QF:27:GLN:HG2   | 6:QF:27:GLN:H      | 1.65                     | 0.43              |
| 7:QG:23:VAL:O     | 7:QG:24:THR:C      | 2.62                     | 0.43              |
| 7:QG:148:ASN:O    | 7:QG:150:ALA:N     | 2.51                     | 0.43              |
| 7:QG:155:ARG:HD3  | 7:QG:155:ARG:H     | 1.83                     | 0.43              |
| 8:QH:28:ALA:O     | 8:QH:29:SER:HB2    | 2.17                     | 0.43              |
| 11:QK:75:TYR:N    | 11:QK:75:TYR:HD1   | 2.17                     | 0.43              |
| 12:QL:76:ASN:O    | 12:QL:76:ASN:CG    | 2.61                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:QM:3:ARG:C      | 13:QM:9:ILE:HG21  | 2.43                     | 0.43              |
| 15:QO:64:ARG:CD    | 15:QO:68:ARG:NH2  | 2.82                     | 0.43              |
| 19:QS:44:MET:HE2   | 19:QS:49:ILE:HD11 | 2.00                     | 0.43              |
| 25:RA:859:G:O2'    | 25:RA:860:U:P     | 2.77                     | 0.43              |
| 25:RA:966:G:C6     | 25:RA:967:C:N4    | 2.87                     | 0.43              |
| 25:RA:2056:G:H2'   | 25:RA:2056:G:N3   | 2.33                     | 0.43              |
| 25:RA:2331:G:O4'   | 46:R0:42:GLY:HA3  | 2.18                     | 0.43              |
| 30:RG:25:TYR:CZ    | 30:RG:32:PRO:HD3  | 2.54                     | 0.43              |
| 30:RG:51:ARG:HB3   | 30:RG:51:ARG:NH1  | 2.33                     | 0.43              |
| 32:RI:29:TYR:HD2   | 32:RI:30:LEU:HD23 | 1.82                     | 0.43              |
| 33:RN:1:MET:HG3    | 33:RN:1:MET:O     | 2.19                     | 0.43              |
| 33:RN:61:ARG:HA    | 33:RN:61:ARG:NE   | 2.33                     | 0.43              |
| 35:RP:135:LEU:HD13 | 35:RP:139:LYS:HE3 | 2.01                     | 0.43              |
| 39:RT:64:ARG:HH11  | 39:RT:64:ARG:HG2  | 1.83                     | 0.43              |
| 39:RT:107:ASP:OD2  | 39:RT:109:GLU:HB2 | 2.18                     | 0.43              |
| 44:RY:26:LYS:O     | 44:RY:27:VAL:C    | 2.62                     | 0.43              |
| 47:R1:44:PRO:O     | 47:R1:46:LEU:N    | 2.51                     | 0.43              |
| 1:XA:93:U:H2'      | 1:XA:95:G:O4'     | 2.19                     | 0.43              |
| 1:XA:947:G:H2'     | 1:XA:948:C:C6     | 2.54                     | 0.43              |
| 1:XA:1015:A:H2'    | 1:XA:1016:A:C8    | 2.53                     | 0.43              |
| 1:XA:1118:C:H1'    | 1:XA:1179:A:C4    | 2.53                     | 0.43              |
| 1:XA:1151:A:H1'    | 10:XJ:39:PRO:CB   | 2.46                     | 0.43              |
| 2:XB:29:ALA:O      | 2:XB:32:ILE:HG22  | 2.17                     | 0.43              |
| 2:XB:32:ILE:HD13   | 2:XB:190:THR:CG2  | 2.48                     | 0.43              |
| 2:XB:127:ILE:HG23  | 2:XB:128:GLU:N    | 2.34                     | 0.43              |
| 3:XC:69:HIS:HA     | 3:XC:104:GLN:HB2  | 2.00                     | 0.43              |
| 4:XD:90:GLY:O      | 4:XD:93:PHE:HB3   | 2.19                     | 0.43              |
| 5:XE:64:ARG:HH11   | 5:XE:64:ARG:HG3   | 1.82                     | 0.43              |
| 5:XE:126:ARG:CG    | 5:XE:126:ARG:NH1  | 2.79                     | 0.43              |
| 6:XF:85:VAL:HG12   | 6:XF:85:VAL:O     | 2.18                     | 0.43              |
| 7:XG:122:HIS:HA    | 7:XG:125:MET:HB2  | 2.00                     | 0.43              |
| 8:XH:29:SER:O      | 8:XH:30:ARG:C     | 2.62                     | 0.43              |
| 9:XI:43:ALA:O      | 9:XI:45:ALA:N     | 2.51                     | 0.43              |
| 10:XJ:70:ARG:HG3   | 10:XJ:70:ARG:HH11 | 1.83                     | 0.43              |
| 10:XJ:90:LEU:N     | 10:XJ:91:PRO:CD   | 2.82                     | 0.43              |
| 11:XK:88:GLY:O     | 11:XK:89:ALA:C    | 2.61                     | 0.43              |
| 13:XM:90:LEU:HD12  | 13:XM:91:ARG:N    | 2.33                     | 0.43              |
| 16:XP:21:VAL:HG23  | 16:XP:34:GLU:N    | 2.34                     | 0.43              |
| 16:XP:39:TYR:CZ    | 16:XP:41:PRO:HB3  | 2.52                     | 0.43              |
| 20:XT:32:ALA:O     | 20:XT:33:ILE:C    | 2.60                     | 0.43              |
| 20:XT:44:ALA:HB1   | 20:XT:91:LEU:HB2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:729:G:N7    | 27:YD:209:ALA:HB3  | 2.34                     | 0.43              |
| 25:YA:2219:G:OP1  | 27:YD:172:TYR:OH   | 2.26                     | 0.43              |
| 25:YA:2630:G:O4'  | 25:YA:2894:G:H1'   | 2.18                     | 0.43              |
| 27:YD:181:GLU:HA  | 27:YD:272:ALA:CB   | 2.39                     | 0.43              |
| 28:YE:155:LYS:O   | 28:YE:156:MET:HG3  | 2.19                     | 0.43              |
| 28:YE:179:GLU:CB  | 28:YE:181:LEU:HD23 | 2.24                     | 0.43              |
| 30:YG:139:LEU:C   | 30:YG:139:LEU:HD12 | 2.43                     | 0.43              |
| 35:YP:144:GLU:N   | 35:YP:144:GLU:CD   | 2.75                     | 0.43              |
| 39:YT:64:ARG:HH11 | 39:YT:64:ARG:HG2   | 1.84                     | 0.43              |
| 40:YU:99:ALA:HA   | 40:YU:106:PHE:HB2  | 2.01                     | 0.43              |
| 44:YY:26:LYS:O    | 44:YY:27:VAL:C     | 2.62                     | 0.43              |
| 47:Y1:44:PRO:O    | 47:Y1:46:LEU:N     | 2.51                     | 0.43              |
| 48:Y2:62:THR:O    | 48:Y2:65:ASN:HB2   | 2.19                     | 0.43              |
| 49:Y3:27:GLY:C    | 49:Y3:28:LEU:HD23  | 2.43                     | 0.43              |
| 54:Y8:28:GLY:O    | 54:Y8:29:LYS:C     | 2.61                     | 0.43              |
| 1:QA:41:G:H2'     | 1:QA:42:G:C8       | 2.54                     | 0.43              |
| 1:QA:691:G:H2'    | 1:QA:692:U:C6      | 2.53                     | 0.43              |
| 1:QA:1069:C:O3'   | 5:QE:25:ARG:NH1    | 2.51                     | 0.43              |
| 1:QA:1211:U:H5'   | 1:QA:1212:U:OP1    | 2.18                     | 0.43              |
| 2:QB:77:ALA:HB1   | 2:QB:165:VAL:HG11  | 2.00                     | 0.43              |
| 3:QC:188:LEU:HD12 | 3:QC:195:VAL:CG1   | 2.48                     | 0.43              |
| 4:QD:90:GLY:O     | 4:QD:93:PHE:HB3    | 2.19                     | 0.43              |
| 6:QF:73:ASN:O     | 6:QF:76:ALA:HB3    | 2.19                     | 0.43              |
| 7:QG:122:HIS:HA   | 7:QG:125:MET:HB2   | 2.00                     | 0.43              |
| 9:QI:26:VAL:CG1   | 9:QI:63:ILE:HD13   | 2.48                     | 0.43              |
| 14:QN:17:LYS:HG3  | 14:QN:18:VAL:N     | 2.33                     | 0.43              |
| 15:QO:83:GLU:HA   | 15:QO:83:GLU:OE1   | 2.18                     | 0.43              |
| 18:QR:29:PHE:N    | 18:QR:29:PHE:HD2   | 2.17                     | 0.43              |
| 22:QV:43:A:H2'    | 22:QV:44:A:C8      | 2.54                     | 0.43              |
| 25:RA:389:G:H22   | 35:RP:72:PRO:CD    | 2.32                     | 0.43              |
| 25:RA:1657:C:H2'  | 25:RA:1658:C:C6    | 2.53                     | 0.43              |
| 25:RA:2552:U:H2'  | 25:RA:2554:U:OP2   | 2.19                     | 0.43              |
| 25:RA:2811:G:H8   | 25:RA:2811:G:OP2   | 2.01                     | 0.43              |
| 26:RB:15:A:H1'    | 26:RB:109:G:C4     | 2.54                     | 0.43              |
| 27:RD:44:ASN:HB3  | 27:RD:49:ILE:CG2   | 2.47                     | 0.43              |
| 27:RD:44:ASN:CB   | 27:RD:49:ILE:HG22  | 2.46                     | 0.43              |
| 27:RD:76:PRO:O    | 27:RD:98:VAL:CG2   | 2.65                     | 0.43              |
| 29:RF:20:LEU:HD12 | 29:RF:21:ALA:N     | 2.25                     | 0.43              |
| 31:RH:6:ARG:CG    | 31:RH:7:LEU:N      | 2.81                     | 0.43              |
| 31:RH:119:GLU:CD  | 31:RH:120:GLY:N    | 2.77                     | 0.43              |
| 35:RP:120:ALA:HB1 | 35:RP:138:LEU:CB   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:RV:27:ALA:O    | 41:RV:28:GLU:C    | 2.61                     | 0.43              |
| 42:RW:1:MET:CB    | 42:RW:64:MET:HE3  | 2.48                     | 0.43              |
| 42:RW:19:LEU:O    | 42:RW:22:ASP:HB2  | 2.19                     | 0.43              |
| 45:RZ:5:LEU:HB3   | 45:RZ:59:LEU:HD23 | 2.01                     | 0.43              |
| 50:R4:59:PHE:CE1  | 50:R4:70:GLY:N    | 2.87                     | 0.43              |
| 53:R7:19:ARG:HG2  | 53:R7:19:ARG:NH1  | 2.33                     | 0.43              |
| 1:XA:19:C:H2'     | 1:XA:20:U:H6      | 1.83                     | 0.43              |
| 1:XA:210:U:O2'    | 1:XA:216:G:N7     | 2.47                     | 0.43              |
| 1:XA:701:C:O2'    | 1:XA:702:A:OP2    | 2.31                     | 0.43              |
| 1:XA:947:G:H4'    | 1:XA:1332:A:H2    | 1.84                     | 0.43              |
| 1:XA:974:A:OP2    | 14:YN:29:ARG:NH2  | 2.52                     | 0.43              |
| 1:XA:992:U:H3     | 1:XA:1044:A:H62   | 1.67                     | 0.43              |
| 2:XB:100:GLY:N    | 2:XB:176:GLU:OE2  | 2.51                     | 0.43              |
| 4:XD:60:GLU:HG2   | 4:XD:202:LEU:HD12 | 2.00                     | 0.43              |
| 4:XD:89:THR:O     | 4:XD:90:GLY:C     | 2.60                     | 0.43              |
| 5:XE:31:LEU:HD22  | 5:XE:31:LEU:HA    | 1.86                     | 0.43              |
| 9:XI:41:VAL:HG12  | 9:XI:41:VAL:O     | 2.18                     | 0.43              |
| 10:XJ:8:LEU:C     | 10:XJ:16:LEU:HD21 | 2.43                     | 0.43              |
| 11:XK:75:TYR:N    | 11:XK:75:TYR:HD1  | 2.16                     | 0.43              |
| 13:XM:54:VAL:O    | 13:XM:58:GLU:OE2  | 2.37                     | 0.43              |
| 15:XO:17:ARG:HD3  | 15:XO:26:GLU:HG3  | 2.01                     | 0.43              |
| 15:XO:71:GLN:HB2  | 15:XO:78:TYR:CE1  | 2.54                     | 0.43              |
| 19:XS:29:ARG:HH11 | 19:XS:29:ARG:HG2  | 1.84                     | 0.43              |
| 25:YA:2756:U:H1'  | 25:YA:2757:A:H5'' | 1.99                     | 0.43              |
| 25:YA:2849:U:H5   | 39:YT:93:ARG:HH12 | 1.67                     | 0.43              |
| 27:YD:172:TYR:HD1 | 27:YD:185:VAL:C   | 2.26                     | 0.43              |
| 28:YE:23:VAL:HG12 | 28:YE:184:VAL:O   | 2.19                     | 0.43              |
| 30:YG:56:ALA:HB2  | 30:YG:153:ARG:NE  | 2.27                     | 0.43              |
| 30:YG:59:GLU:O    | 30:YG:62:LEU:HB3  | 2.18                     | 0.43              |
| 31:YH:119:GLU:CD  | 31:YH:120:GLY:N   | 2.77                     | 0.43              |
| 36:YQ:27:VAL:HG13 | 36:YQ:28:ALA:N    | 2.32                     | 0.43              |
| 39:YT:19:LEU:HA   | 39:YT:20:PRO:HD3  | 1.88                     | 0.43              |
| 39:YT:89:VAL:O    | 39:YT:90:GLN:CB   | 2.67                     | 0.43              |
| 40:YU:53:ARG:C    | 40:YU:55:ARG:N    | 2.77                     | 0.43              |
| 44:YY:47:LYS:O    | 44:YY:49:VAL:N    | 2.48                     | 0.43              |
| 45:YZ:157:LEU:HA  | 45:YZ:158:PRO:HD2 | 1.92                     | 0.43              |
| 47:Y1:29:GLY:O    | 47:Y1:31:GLY:N    | 2.49                     | 0.43              |
| 49:Y3:50:VAL:HB   | 49:Y3:53:LEU:HD12 | 2.00                     | 0.43              |
| 1:QA:458:C:H2'    | 1:QA:464:G:H8     | 1.84                     | 0.43              |
| 1:QA:590:C:OP1    | 8:QH:29:SER:HA    | 2.19                     | 0.43              |
| 1:QA:1346:A:H5'   | 9:QI:120:ARG:HH12 | 1.84                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:QB:54:THR:HG21   | 2:QB:201:ILE:HD11 | 2.00                     | 0.43              |
| 2:QB:95:GLN:HE21   | 2:QB:147:LYS:CE   | 2.28                     | 0.43              |
| 4:QD:52:SER:O      | 4:QD:55:ALA:N     | 2.52                     | 0.43              |
| 5:QE:105:VAL:HB    | 5:QE:106:PRO:CD   | 2.49                     | 0.43              |
| 5:QE:152:ARG:O     | 8:QH:64:LYS:NZ    | 2.51                     | 0.43              |
| 8:QH:20:TYR:CD1    | 8:QH:65:TYR:HD2   | 2.35                     | 0.43              |
| 8:QH:64:LYS:CB     | 8:QH:79:VAL:HG21  | 2.49                     | 0.43              |
| 10:QJ:75:ILE:CG1   | 10:QJ:76:ASN:H    | 2.17                     | 0.43              |
| 11:QK:44:SER:O     | 11:QK:48:ILE:HG12 | 2.18                     | 0.43              |
| 11:QK:108:ILE:HG21 | 18:QR:88:LYS:OXT  | 2.18                     | 0.43              |
| 13:QM:77:ASN:HA    | 50:R4:71:ARG:CZ   | 2.47                     | 0.43              |
| 13:QM:77:ASN:O     | 13:QM:78:ILE:C    | 2.62                     | 0.43              |
| 25:RA:155:C:H5'    | 25:RA:161:U:OP2   | 2.19                     | 0.43              |
| 25:RA:1181:C:H2'   | 25:RA:1182:A:H8   | 1.83                     | 0.43              |
| 25:RA:2540:C:H2'   | 25:RA:2541:A:O4'  | 2.17                     | 0.43              |
| 25:RA:2832:U:O2'   | 25:RA:2833:G:P    | 2.77                     | 0.43              |
| 28:RE:48:GLN:HE21  | 28:RE:48:GLN:HB3  | 1.55                     | 0.43              |
| 29:RF:64:ILE:HG23  | 29:RF:65:TRP:CD1  | 2.54                     | 0.43              |
| 29:RF:176:LEU:HD11 | 29:RF:180:GLY:O   | 2.19                     | 0.43              |
| 30:RG:4:ASP:O      | 30:RG:5:VAL:HB    | 2.19                     | 0.43              |
| 34:RO:17:ARG:HH11  | 34:RO:17:ARG:HG2  | 1.84                     | 0.43              |
| 34:RO:61:VAL:O     | 34:RO:61:VAL:HG13 | 2.18                     | 0.43              |
| 34:RO:112:MET:O    | 34:RO:113:LYS:C   | 2.60                     | 0.43              |
| 34:RO:112:MET:HE2  | 34:RO:112:MET:N   | 2.34                     | 0.43              |
| 35:RP:52:GLU:OE2   | 35:RP:58:THR:N    | 2.52                     | 0.43              |
| 37:RR:10:LEU:O     | 37:RR:12:ARG:N    | 2.52                     | 0.43              |
| 38:RS:18:ILE:O     | 38:RS:19:LYS:C    | 2.62                     | 0.43              |
| 38:RS:110:LEU:HA   | 38:RS:112:PHE:CZ  | 2.53                     | 0.43              |
| 40:RU:53:ARG:C     | 40:RU:55:ARG:N    | 2.77                     | 0.43              |
| 40:RU:90:VAL:C     | 40:RU:92:ARG:N    | 2.76                     | 0.43              |
| 41:RV:72:VAL:HG13  | 41:RV:72:VAL:O    | 2.19                     | 0.43              |
| 42:RW:28:SER:O     | 42:RW:30:GLU:N    | 2.50                     | 0.43              |
| 42:RW:111:HIS:CG   | 42:RW:112:GLY:H   | 2.37                     | 0.43              |
| 53:R7:17:GLY:O     | 53:R7:20:ALA:HB3  | 2.18                     | 0.43              |
| 54:R8:28:GLY:O     | 54:R8:29:LYS:O    | 2.36                     | 0.43              |
| 1:XA:1010:G:H2'    | 1:XA:1011:G:C8    | 2.53                     | 0.43              |
| 1:XA:1366:C:H2'    | 1:XA:1367:C:C6    | 2.54                     | 0.43              |
| 2:XB:69:LEU:HD12   | 2:XB:91:PRO:O     | 2.19                     | 0.43              |
| 2:XB:130:ARG:NH2   | 2:XB:138:LEU:HD21 | 2.34                     | 0.43              |
| 4:XD:59:ARG:NE     | 4:XD:59:ARG:HA    | 2.34                     | 0.43              |
| 4:XD:72:GLU:O      | 4:XD:73:ARG:C     | 2.61                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:XF:45:LEU:CD1    | 6:XF:59:TYR:HD1    | 2.30                     | 0.43              |
| 7:XG:23:VAL:O      | 7:XG:27:ILE:HD12   | 2.19                     | 0.43              |
| 7:XG:79:ARG:NH1    | 7:XG:82:GLY:HA2    | 2.34                     | 0.43              |
| 7:XG:79:ARG:HH12   | 7:XG:82:GLY:HA2    | 1.84                     | 0.43              |
| 8:XH:64:LYS:CB     | 8:XH:79:VAL:HG21   | 2.48                     | 0.43              |
| 8:XH:86:ILE:CB     | 8:XH:133:LEU:HD22  | 2.49                     | 0.43              |
| 8:XH:118:VAL:O     | 8:XH:119:LEU:HD23  | 2.18                     | 0.43              |
| 9:XI:17:VAL:HG21   | 9:XI:80:GLY:C      | 2.44                     | 0.43              |
| 9:XI:26:VAL:CG1    | 9:XI:63:ILE:HD13   | 2.48                     | 0.43              |
| 10:XJ:10:GLY:O     | 10:XJ:68:HIS:N     | 2.51                     | 0.43              |
| 10:XJ:30:SER:OG    | 10:XJ:81:THR:HG22  | 2.19                     | 0.43              |
| 11:XK:34:ASP:OD1   | 11:XK:38:ASN:HB2   | 2.18                     | 0.43              |
| 11:XK:72:ALA:C     | 11:XK:74:ALA:H     | 2.27                     | 0.43              |
| 11:XK:105:VAL:O    | 11:XK:105:VAL:HG23 | 2.19                     | 0.43              |
| 23:XY:29:U:H2'     | 23:XY:30:C:H6      | 1.84                     | 0.43              |
| 25:YA:531:C:H4'    | 25:YA:532:A:H5''   | 2.00                     | 0.43              |
| 25:YA:608:A:C4     | 25:YA:621:A:C6     | 3.07                     | 0.43              |
| 25:YA:627:A:H4'    | 25:YA:628:G:H5'    | 1.99                     | 0.43              |
| 25:YA:747:U:N3     | 51:Y5:2:ALA:N      | 2.67                     | 0.43              |
| 25:YA:2078:C:C4    | 25:YA:2079:U:C4    | 3.06                     | 0.43              |
| 25:YA:2247:A:H2'   | 25:YA:2248:C:C6    | 2.53                     | 0.43              |
| 26:YB:73:A:C4      | 26:YB:104:A:C2     | 3.07                     | 0.43              |
| 27:YD:117:VAL:HG21 | 27:YD:128:GLY:C    | 2.44                     | 0.43              |
| 28:YE:52:LEU:O     | 28:YE:74:PRO:HA    | 2.18                     | 0.43              |
| 30:YG:31:VAL:O     | 30:YG:31:VAL:HG13  | 2.18                     | 0.43              |
| 30:YG:53:LEU:C     | 30:YG:55:LYS:H     | 2.27                     | 0.43              |
| 31:YH:27:LYS:HD2   | 31:YH:27:LYS:C     | 2.44                     | 0.43              |
| 31:YH:58:GLU:O     | 31:YH:59:ARG:C     | 2.61                     | 0.43              |
| 31:YH:120:GLY:O    | 31:YH:136:ILE:HD12 | 2.19                     | 0.43              |
| 31:YH:125:VAL:CG1  | 31:YH:126:PRO:CG   | 2.94                     | 0.43              |
| 37:YR:51:LEU:HD13  | 37:YR:66:VAL:HG22  | 2.01                     | 0.43              |
| 40:YU:43:GLY:HA3   | 41:YV:73:SER:OG    | 2.19                     | 0.43              |
| 45:YZ:13:GLU:HB3   | 45:YZ:18:LEU:HD11  | 2.00                     | 0.43              |
| 51:Y5:40:LYS:HE2   | 51:Y5:47:PRO:CG    | 2.49                     | 0.43              |
| 1:QA:410:G:H2'     | 1:QA:429:U:C5      | 2.54                     | 0.43              |
| 1:QA:595:G:H8      | 1:QA:595:G:O5'     | 2.02                     | 0.43              |
| 1:QA:792:A:H1'     | 1:QA:793:U:OP2     | 2.19                     | 0.43              |
| 1:QA:868:C:H2'     | 1:QA:869:G:O4'     | 2.19                     | 0.43              |
| 1:QA:978:A:H5''    | 1:QA:979:C:OP2     | 2.19                     | 0.43              |
| 1:QA:1314:C:C5     | 19:QS:4:SER:HB2    | 2.54                     | 0.43              |
| 2:QB:127:ILE:HG23  | 2:QB:128:GLU:N     | 2.34                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:QB:188:ALA:CB    | 2:QB:200:ILE:HG23 | 2.48                     | 0.43              |
| 4:QD:13:ARG:HA     | 4:QD:33:MET:CE    | 2.44                     | 0.43              |
| 4:QD:25:ARG:NH1    | 4:QD:30:LYS:CE    | 2.75                     | 0.43              |
| 5:QE:48:ALA:HB2    | 5:QE:57:LYS:HD3   | 2.00                     | 0.43              |
| 6:QF:22:GLU:OE1    | 6:QF:82:ARG:NH2   | 2.46                     | 0.43              |
| 6:QF:69:GLU:C      | 6:QF:71:ARG:N     | 2.77                     | 0.43              |
| 6:QF:85:VAL:HG12   | 6:QF:85:VAL:O     | 2.18                     | 0.43              |
| 8:QH:91:ARG:HH11   | 8:QH:91:ARG:CG    | 2.23                     | 0.43              |
| 9:QI:17:VAL:HG21   | 9:QI:80:GLY:C     | 2.44                     | 0.43              |
| 16:QP:20:VAL:CG2   | 16:QP:21:VAL:N    | 2.81                     | 0.43              |
| 17:QQ:22:LEU:HD13  | 17:QQ:41:LYS:HG2  | 2.01                     | 0.43              |
| 19:QS:8:GLY:O      | 19:QS:9:VAL:CG2   | 2.57                     | 0.43              |
| 25:RA:443:A:H1'    | 25:RA:1201:C:O4'  | 2.19                     | 0.43              |
| 25:RA:631:A:P      | 54:R8:46:ARG:HH21 | 2.40                     | 0.43              |
| 25:RA:974(A):C:H4' | 25:RA:975:G:O5'   | 2.18                     | 0.43              |
| 25:RA:1278:A:H2'   | 25:RA:1279:G:C8   | 2.54                     | 0.43              |
| 25:RA:1430:C:H2'   | 25:RA:1431:U:H6   | 1.83                     | 0.43              |
| 25:RA:1889:A:N1    | 25:RA:2234:G:H1'  | 2.34                     | 0.43              |
| 25:RA:2252:G:H2'   | 25:RA:2253:G:O4'  | 2.19                     | 0.43              |
| 29:RF:65:TRP:HZ3   | 29:RF:73:ALA:C    | 2.26                     | 0.43              |
| 30:RG:31:VAL:O     | 30:RG:31:VAL:HG13 | 2.18                     | 0.43              |
| 31:RH:16:SER:OG    | 31:RH:17:VAL:N    | 2.50                     | 0.43              |
| 35:RP:19:VAL:HG22  | 35:RP:21:ARG:H    | 1.83                     | 0.43              |
| 35:RP:49:ARG:HG2   | 35:RP:49:ARG:HH11 | 1.84                     | 0.43              |
| 38:RS:52:SER:HB2   | 38:RS:55:ALA:CB   | 2.49                     | 0.43              |
| 40:RU:27:LEU:O     | 40:RU:28:ARG:C    | 2.61                     | 0.43              |
| 41:RV:36:PRO:HA    | 41:RV:56:SER:HG   | 1.84                     | 0.43              |
| 47:R1:13:ILE:CG1   | 47:R1:42:GLN:HB2  | 2.49                     | 0.43              |
| 47:R1:29:GLY:C     | 47:R1:30:VAL:HG23 | 2.43                     | 0.43              |
| 49:R3:27:GLY:C     | 49:R3:28:LEU:HD23 | 2.43                     | 0.43              |
| 50:R4:43:TYR:O     | 50:R4:46:GLN:HA   | 2.19                     | 0.43              |
| 50:R4:48:ARG:NH1   | 50:R4:51:ASP:HA   | 2.34                     | 0.43              |
| 55:R9:1:MET:HE2    | 55:R9:10:ILE:CD1  | 2.49                     | 0.43              |
| 1:XA:538:G:O3'     | 12:XL:114:LYS:HD3 | 2.19                     | 0.43              |
| 1:XA:655:A:H61     | 1:XA:751:U:H3     | 1.67                     | 0.43              |
| 1:XA:676:A:H1'     | 11:XK:115:PRO:HB3 | 2.01                     | 0.43              |
| 1:XA:986:A:H1'     | 19:XS:54:GLY:O    | 2.18                     | 0.43              |
| 1:XA:1034:G:H2'    | 1:XA:1035:A:C8    | 2.53                     | 0.43              |
| 2:XB:17:PHE:CG     | 2:XB:44:LEU:HD11  | 2.53                     | 0.43              |
| 2:XB:87:ARG:NH1    | 2:XB:223:ILE:HD12 | 2.33                     | 0.43              |
| 2:XB:197:VAL:CG1   | 2:XB:198:ASP:N    | 2.82                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:XC:67:THR:O      | 3:XC:69:HIS:CE1    | 2.72                     | 0.43              |
| 4:XD:90:GLY:HA3    | 4:XD:204:ILE:HD11  | 2.01                     | 0.43              |
| 5:XE:105:VAL:HB    | 5:XE:106:PRO:CD    | 2.49                     | 0.43              |
| 8:XH:20:TYR:CD1    | 8:XH:65:TYR:HD2    | 2.35                     | 0.43              |
| 10:XJ:74:ILE:H     | 10:XJ:74:ILE:CD1   | 2.21                     | 0.43              |
| 11:XK:44:SER:O     | 11:XK:48:ILE:HG12  | 2.18                     | 0.43              |
| 19:XS:44:MET:HE2   | 19:XS:49:ILE:HD11  | 2.00                     | 0.43              |
| 19:XS:51:VAL:HG12  | 19:XS:52:TYR:N     | 2.33                     | 0.43              |
| 22:XV:53:G:HO2'    | 22:XV:54:U:H6      | 1.66                     | 0.43              |
| 25:YA:601:C:O2'    | 25:YA:605:C:H5''   | 2.19                     | 0.43              |
| 25:YA:1512:G:H2'   | 25:YA:1513:C:C6    | 2.53                     | 0.43              |
| 25:YA:2070:G:C2    | 25:YA:2071:A:C4    | 3.07                     | 0.43              |
| 26:YB:44:G:H1'     | 26:YB:47:C:N4      | 2.34                     | 0.43              |
| 30:YG:139:LEU:HA   | 30:YG:144:ILE:HG21 | 2.00                     | 0.43              |
| 35:YP:26:GLY:C     | 35:YP:28:GLY:H     | 2.26                     | 0.43              |
| 35:YP:101:VAL:HG13 | 35:YP:102:ARG:N    | 2.33                     | 0.43              |
| 36:YQ:57:HIS:ND1   | 36:YQ:58:PHE:N     | 2.67                     | 0.43              |
| 37:YR:94:TYR:N     | 37:YR:94:TYR:CD2   | 2.87                     | 0.43              |
| 42:YW:65:LEU:CD1   | 42:YW:68:ARG:NH1   | 2.75                     | 0.43              |
| 47:Y1:53:VAL:CG1   | 47:Y1:54:ALA:N     | 2.81                     | 0.43              |
| 53:Y7:5:TRP:CD1    | 53:Y7:7:PRO:HG3    | 2.53                     | 0.43              |
| 1:QA:595:G:H1'     | 1:QA:596:C:C5      | 2.53                     | 0.42              |
| 1:QA:986:A:H2'     | 1:QA:987:G:O4'     | 2.18                     | 0.42              |
| 1:QA:1158:C:H4'    | 2:QB:133:LYS:NZ    | 2.32                     | 0.42              |
| 1:QA:1321:C:H4'    | 13:QM:87:TYR:CE2   | 2.54                     | 0.42              |
| 1:QA:1327:C:H2'    | 1:QA:1328:C:H6     | 1.84                     | 0.42              |
| 2:QB:162:ILE:O     | 2:QB:185:ILE:HG13  | 2.19                     | 0.42              |
| 3:QC:22:TRP:CB     | 3:QC:59:ARG:HB2    | 2.48                     | 0.42              |
| 3:QC:76:VAL:CG2    | 3:QC:103:VAL:HG11  | 2.49                     | 0.42              |
| 3:QC:83:ARG:O      | 3:QC:86:VAL:HG22   | 2.19                     | 0.42              |
| 5:QE:126:ARG:NH1   | 5:QE:126:ARG:CG    | 2.79                     | 0.42              |
| 6:QF:23:LYS:HG2    | 6:QF:27:GLN:OE1    | 2.18                     | 0.42              |
| 7:QG:6:ARG:O       | 7:QG:7:ALA:C       | 2.62                     | 0.42              |
| 13:QM:87:TYR:HA    | 13:QM:90:LEU:HG    | 2.01                     | 0.42              |
| 14:QN:24:CYS:SG    | 14:QN:39:LEU:C     | 3.02                     | 0.42              |
| 16:QP:12:LYS:HB3   | 16:QP:12:LYS:HE2   | 1.73                     | 0.42              |
| 18:QR:40:LEU:C     | 18:QR:42:ARG:N     | 2.76                     | 0.42              |
| 18:QR:73:ALA:HB3   | 18:QR:79:LEU:CD1   | 2.47                     | 0.42              |
| 18:QR:74:ARG:NH2   | 18:QR:81:PHE:HA    | 2.34                     | 0.42              |
| 19:QS:29:ARG:HH11  | 19:QS:29:ARG:HG2   | 1.84                     | 0.42              |
| 19:QS:30:LEU:C     | 19:QS:30:LEU:HD22  | 2.44                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:QT:81:LYS:C     | 20:QT:83:ARG:H     | 2.27                     | 0.42              |
| 23:QY:29:U:H2'     | 23:QY:30:C:H6      | 1.84                     | 0.42              |
| 25:RA:572:A:H5''   | 25:RA:573:G:OP2    | 2.19                     | 0.42              |
| 25:RA:811:U:O2'    | 35:RP:21:ARG:HG3   | 2.19                     | 0.42              |
| 25:RA:1024:G:C6    | 25:RA:1025:G:C6    | 3.06                     | 0.42              |
| 25:RA:1045:A:N3    | 25:RA:1047:G:N2    | 2.67                     | 0.42              |
| 25:RA:1510:A:O2'   | 25:RA:1511:A:N7    | 2.51                     | 0.42              |
| 25:RA:2377:A:H2'   | 25:RA:2378:A:C8    | 2.54                     | 0.42              |
| 25:RA:2481:G:O2'   | 25:RA:2482:G:P     | 2.77                     | 0.42              |
| 25:RA:2779:U:O2'   | 25:RA:2781:A:N7    | 2.52                     | 0.42              |
| 27:RD:71:ASP:CB    | 27:RD:103:ARG:HH22 | 2.32                     | 0.42              |
| 27:RD:108:PRO:HG2  | 27:RD:111:LEU:HB2  | 2.01                     | 0.42              |
| 27:RD:117:VAL:HG21 | 27:RD:128:GLY:C    | 2.44                     | 0.42              |
| 28:RE:25:VAL:HG21  | 39:RT:8:LYS:HG3    | 2.00                     | 0.42              |
| 28:RE:188:VAL:HA   | 28:RE:189:PRO:HD2  | 1.79                     | 0.42              |
| 30:RG:83:ARG:CG    | 30:RG:86:MET:HE3   | 2.49                     | 0.42              |
| 33:RN:63:THR:HG23  | 33:RN:66:LYS:HE3   | 2.00                     | 0.42              |
| 34:RO:31:LYS:O     | 34:RO:32:TYR:HD2   | 2.02                     | 0.42              |
| 35:RP:112:LEU:CD1  | 35:RP:114:ILE:HG23 | 2.47                     | 0.42              |
| 37:RR:51:LEU:HD13  | 37:RR:66:VAL:HG22  | 2.01                     | 0.42              |
| 40:RU:27:LEU:O     | 40:RU:30:LYS:N     | 2.41                     | 0.42              |
| 40:RU:98:LEU:O     | 40:RU:102:GLU:N    | 2.49                     | 0.42              |
| 41:RV:44:LYS:C     | 41:RV:46:VAL:N     | 2.77                     | 0.42              |
| 45:RZ:177:PRO:HB2  | 45:RZ:178:GLU:H    | 1.64                     | 0.42              |
| 48:R2:62:THR:O     | 48:R2:65:ASN:HB2   | 2.19                     | 0.42              |
| 52:R6:50:ARG:HH11  | 52:R6:50:ARG:HG2   | 1.84                     | 0.42              |
| 1:XA:1053:G:N7     | 1:XA:1199:U:H3'    | 2.34                     | 0.42              |
| 1:XA:1128:C:H42    | 1:XA:1144:G:H1     | 1.66                     | 0.42              |
| 1:XA:1190:G:P      | 3:XC:5:ILE:HG23    | 2.58                     | 0.42              |
| 1:XA:1346:A:C4     | 7:XG:10:ARG:NH1    | 2.88                     | 0.42              |
| 3:XC:125:GLU:CD    | 3:XC:189:ALA:HA    | 2.44                     | 0.42              |
| 4:XD:10:ARG:HG3    | 4:XD:10:ARG:NH1    | 2.33                     | 0.42              |
| 4:XD:88:VAL:O      | 4:XD:89:THR:C      | 2.62                     | 0.42              |
| 5:XE:56:GLN:C      | 5:XE:58:ALA:N      | 2.77                     | 0.42              |
| 6:XF:3:ARG:HB3     | 6:XF:93:SER:CB     | 2.48                     | 0.42              |
| 9:XI:25:LYS:O      | 9:XI:60:ASP:OD1    | 2.37                     | 0.42              |
| 13:XM:3:ARG:HD2    | 13:XM:9:ILE:CG1    | 2.45                     | 0.42              |
| 14:XN:44:LEU:CD1   | 14:XN:48:ALA:HB2   | 2.47                     | 0.42              |
| 16:XP:20:VAL:CG2   | 16:XP:21:VAL:N     | 2.82                     | 0.42              |
| 17:XQ:13:ASP:C     | 17:XQ:15:MET:N     | 2.77                     | 0.42              |
| 20:XT:96:GLY:O     | 20:XT:99:LEU:CD1   | 2.67                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:219:G:N3    | 25:YA:234:C:O2'    | 2.48                     | 0.42              |
| 25:YA:467:G:OP1   | 53:Y7:33:ARG:NH1   | 2.51                     | 0.42              |
| 25:YA:2068:U:N3   | 25:YA:2430:A:H2    | 2.03                     | 0.42              |
| 25:YA:2655:G:N2   | 25:YA:2665:A:OP2   | 2.52                     | 0.42              |
| 27:YD:17:THR:HG22 | 27:YD:204:ILE:HA   | 1.98                     | 0.42              |
| 29:YF:45:ARG:HH11 | 29:YF:45:ARG:HG2   | 1.82                     | 0.42              |
| 29:YF:63:LYS:CE   | 29:YF:67:GLN:HB2   | 2.49                     | 0.42              |
| 29:YF:64:ILE:HD12 | 29:YF:64:ILE:HA    | 1.89                     | 0.42              |
| 29:YF:135:LYS:O   | 29:YF:136:THR:C    | 2.61                     | 0.42              |
| 30:YG:25:TYR:CZ   | 30:YG:32:PRO:HD3   | 2.54                     | 0.42              |
| 33:YN:57:ALA:O    | 33:YN:124:ALA:HA   | 2.18                     | 0.42              |
| 34:YO:78:ARG:HH21 | 39:YT:103:ARG:HH22 | 1.64                     | 0.42              |
| 35:YP:81:GLN:HE21 | 35:YP:81:GLN:HB2   | 1.59                     | 0.42              |
| 37:YR:81:ASP:N    | 37:YR:81:ASP:OD2   | 2.51                     | 0.42              |
| 41:YV:38:LEU:CD2  | 41:YV:39:LEU:N     | 2.82                     | 0.42              |
| 47:Y1:8:SER:CB    | 47:Y1:66:HIS:CE1   | 3.01                     | 0.42              |
| 48:Y2:48:HIS:C    | 48:Y2:50:ILE:N     | 2.76                     | 0.42              |
| 53:Y7:47:ARG:HB2  | 53:Y7:48:LYS:H     | 1.64                     | 0.42              |
| 1:QA:942:G:C2     | 1:QA:1342:C:C2     | 3.07                     | 0.42              |
| 1:QA:1126:U:H1'   | 1:QA:1280:A:N7     | 2.35                     | 0.42              |
| 1:QA:1442:G:C5    | 1:QA:1446:A:C6     | 3.07                     | 0.42              |
| 2:QB:95:GLN:HB3   | 2:QB:148:TYR:HD1   | 1.84                     | 0.42              |
| 2:QB:136:VAL:O    | 2:QB:140:HIS:N     | 2.44                     | 0.42              |
| 2:QB:211:ILE:O    | 2:QB:215:LEU:HB2   | 2.19                     | 0.42              |
| 4:QD:22:LYS:CD    | 4:QD:26:CYS:SG     | 3.05                     | 0.42              |
| 4:QD:128:VAL:C    | 4:QD:130:GLY:N     | 2.76                     | 0.42              |
| 7:QG:75:VAL:HG13  | 7:QG:145:ALA:HA    | 2.00                     | 0.42              |
| 9:QI:29:ASN:OD1   | 9:QI:65:VAL:N      | 2.48                     | 0.42              |
| 10:QJ:30:SER:OG   | 10:QJ:81:THR:HG22  | 2.19                     | 0.42              |
| 13:QM:4:ILE:CG2   | 13:QM:5:ALA:H      | 2.29                     | 0.42              |
| 15:QO:8:LYS:NZ    | 15:QO:31:LEU:HD11  | 2.34                     | 0.42              |
| 15:QO:17:ARG:HD3  | 15:QO:26:GLU:HG3   | 2.00                     | 0.42              |
| 15:QO:25:THR:O    | 15:QO:29:VAL:HG23  | 2.18                     | 0.42              |
| 17:QQ:77:VAL:O    | 17:QQ:78:GLU:HB2   | 2.18                     | 0.42              |
| 19:QS:62:ILE:HG22 | 19:QS:63:THR:N     | 2.34                     | 0.42              |
| 25:RA:1340:U:OP2  | 43:RX:78:LYS:NZ    | 2.45                     | 0.42              |
| 25:RA:1538:G:H2'  | 25:RA:1539:G:H8    | 1.83                     | 0.42              |
| 27:RD:17:THR:HG21 | 27:RD:204:ILE:HA   | 1.99                     | 0.42              |
| 27:RD:134:ARG:H   | 27:RD:134:ARG:HG3  | 1.55                     | 0.42              |
| 28:RE:23:VAL:HG12 | 28:RE:184:VAL:O    | 2.19                     | 0.42              |
| 28:RE:155:LYS:O   | 28:RE:156:MET:HG3  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:114:ILE:O    | 30:RG:116:ASP:N    | 2.51                     | 0.42              |
| 30:RG:145:THR:O    | 30:RG:146:TYR:HB3  | 2.19                     | 0.42              |
| 33:RN:7:LYS:HD2    | 33:RN:7:LYS:N      | 2.29                     | 0.42              |
| 33:RN:10:GLU:OE2   | 33:RN:11:PRO:CD    | 2.67                     | 0.42              |
| 34:RO:2:ILE:N      | 34:RO:2:ILE:CD1    | 2.82                     | 0.42              |
| 35:RP:26:GLY:C     | 35:RP:28:GLY:H     | 2.27                     | 0.42              |
| 35:RP:114:ILE:CD1  | 35:RP:130:PHE:CE1  | 2.98                     | 0.42              |
| 37:RR:44:LEU:HD23  | 37:RR:44:LEU:HA    | 1.79                     | 0.42              |
| 40:RU:81:HIS:O     | 40:RU:82:GLY:C     | 2.61                     | 0.42              |
| 42:RW:88:ARG:CB    | 42:RW:92:ARG:HB3   | 2.47                     | 0.42              |
| 47:R1:29:GLY:C     | 47:R1:31:GLY:H     | 2.26                     | 0.42              |
| 47:R1:60:PHE:HE2   | 47:R1:91:LYS:NZ    | 2.16                     | 0.42              |
| 51:R5:3:LYS:HA     | 51:R5:3:LYS:CE     | 2.36                     | 0.42              |
| 52:R6:7:ILE:O      | 52:R6:8:LYS:CG     | 2.68                     | 0.42              |
| 53:R7:47:ARG:HB2   | 53:R7:48:LYS:H     | 1.64                     | 0.42              |
| 1:XA:35:G:H2'      | 1:XA:36:C:C6       | 2.55                     | 0.42              |
| 1:XA:690:G:H22     | 11:XK:55:LYS:NZ    | 2.16                     | 0.42              |
| 1:XA:1442:G:C5     | 1:XA:1446:A:C6     | 3.07                     | 0.42              |
| 2:XB:44:LEU:H      | 2:XB:44:LEU:CD1    | 2.26                     | 0.42              |
| 2:XB:142:LEU:HD23  | 2:XB:142:LEU:O     | 2.18                     | 0.42              |
| 2:XB:142:LEU:O     | 2:XB:145:LEU:HB2   | 2.19                     | 0.42              |
| 4:XD:120:LEU:HD23  | 4:XD:120:LEU:HA    | 1.83                     | 0.42              |
| 11:XK:62:GLN:O     | 11:XK:64:ALA:N     | 2.52                     | 0.42              |
| 17:XQ:77:VAL:O     | 17:XQ:78:GLU:HB2   | 2.18                     | 0.42              |
| 19:XS:18:LYS:O     | 19:XS:18:LYS:HD2   | 2.19                     | 0.42              |
| 19:XS:39:THR:CG2   | 19:XS:40:ILE:H     | 2.23                     | 0.42              |
| 22:XV:4:G:C6       | 22:XV:70:G:N1      | 2.86                     | 0.42              |
| 25:YA:236:C:H2'    | 25:YA:237:C:C6     | 2.54                     | 0.42              |
| 25:YA:2376:A:H2'   | 25:YA:2377:A:O4'   | 2.19                     | 0.42              |
| 27:YD:155:LEU:HD23 | 27:YD:177:LEU:HD21 | 2.00                     | 0.42              |
| 30:YG:7:LEU:CD2    | 30:YG:176:LEU:HD22 | 2.45                     | 0.42              |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CD   | 2.49                     | 0.42              |
| 33:YN:62:VAL:HG12  | 33:YN:66:LYS:HB2   | 2.02                     | 0.42              |
| 35:YP:120:ALA:HB1  | 35:YP:138:LEU:CB   | 2.49                     | 0.42              |
| 37:YR:10:LEU:O     | 37:YR:12:ARG:N     | 2.52                     | 0.42              |
| 38:YS:64:GLU:O     | 38:YS:68:GLN:HG3   | 2.19                     | 0.42              |
| 42:YW:19:LEU:O     | 42:YW:22:ASP:HB2   | 2.19                     | 0.42              |
| 44:YY:60:PHE:CD2   | 44:YY:60:PHE:N     | 2.87                     | 0.42              |
| 47:Y1:13:ILE:CG1   | 47:Y1:42:GLN:HB2   | 2.49                     | 0.42              |
| 49:Y3:46:ASN:O     | 49:Y3:50:VAL:HG22  | 2.19                     | 0.42              |
| 50:Y4:45:GLY:O     | 50:Y4:46:GLN:C     | 2.62                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:Y8:53:PRO:HD2  | 54:Y8:54:GLU:H     | 1.84                     | 0.42              |
| 1:QA:310:G:H4'    | 16:QP:31:LYS:HD3   | 2.00                     | 0.42              |
| 2:QB:16:HIS:CD2   | 2:QB:213:LEU:HD13  | 2.54                     | 0.42              |
| 2:QB:99:GLY:O     | 2:QB:108:ILE:HD11  | 2.20                     | 0.42              |
| 3:QC:125:GLU:CD   | 3:QC:189:ALA:HA    | 2.44                     | 0.42              |
| 3:QC:149:ALA:O    | 3:QC:169:ALA:CA    | 2.67                     | 0.42              |
| 4:QD:89:THR:O     | 4:QD:90:GLY:C      | 2.60                     | 0.42              |
| 5:QE:154:GLY:O    | 5:QE:155:GLU:C     | 2.61                     | 0.42              |
| 7:QG:79:ARG:HH12  | 7:QG:82:GLY:HA2    | 1.84                     | 0.42              |
| 7:QG:126:ASP:N    | 7:QG:126:ASP:OD2   | 2.53                     | 0.42              |
| 10:QJ:49:VAL:HG13 | 10:QJ:50:ILE:N     | 2.35                     | 0.42              |
| 11:QK:124:LYS:HB3 | 11:QK:125:PHE:H    | 1.67                     | 0.42              |
| 18:QR:21:LYS:O    | 18:QR:22:VAL:C     | 2.62                     | 0.42              |
| 19:QS:29:ARG:HD3  | 19:QS:30:LEU:H     | 1.83                     | 0.42              |
| 19:QS:66:MET:O    | 19:QS:66:MET:HG3   | 2.19                     | 0.42              |
| 25:RA:195:A:H61   | 25:RA:198:C:H3'    | 1.84                     | 0.42              |
| 25:RA:1615:C:C2   | 42:RW:87:PRO:HG3   | 2.54                     | 0.42              |
| 25:RA:2758:A:H2'  | 25:RA:2759:G:O4'   | 2.19                     | 0.42              |
| 27:RD:33:LEU:O    | 27:RD:35:LYS:N     | 2.52                     | 0.42              |
| 28:RE:76:ARG:C    | 28:RE:78:LEU:N     | 2.76                     | 0.42              |
| 29:RF:135:LYS:O   | 29:RF:136:THR:C    | 2.62                     | 0.42              |
| 30:RG:41:GLN:NE2  | 30:RG:154:GLY:O    | 2.52                     | 0.42              |
| 33:RN:30:ILE:HG22 | 33:RN:34:LEU:HD21  | 2.01                     | 0.42              |
| 36:RQ:135:ASP:CG  | 45:RZ:81:ARG:HH12  | 2.28                     | 0.42              |
| 39:RT:24:PRO:HA   | 39:RT:49:VAL:CG1   | 2.39                     | 0.42              |
| 39:RT:50:ILE:HD11 | 39:RT:102:ILE:HG12 | 2.01                     | 0.42              |
| 40:RU:91:ASP:O    | 40:RU:95:LEU:N     | 2.43                     | 0.42              |
| 41:RV:29:PRO:C    | 41:RV:61:VAL:HG22  | 2.44                     | 0.42              |
| 41:RV:44:LYS:HB3  | 41:RV:45:THR:H     | 1.56                     | 0.42              |
| 42:RW:8:ARG:HG3   | 42:RW:8:ARG:NH1    | 2.34                     | 0.42              |
| 44:RY:42:VAL:HG11 | 44:RY:65:ALA:HB3   | 2.02                     | 0.42              |
| 48:R2:59:ARG:O    | 48:R2:62:THR:HG23  | 2.18                     | 0.42              |
| 49:R3:39:ASP:O    | 49:R3:39:ASP:CG    | 2.62                     | 0.42              |
| 50:R4:35:VAL:C    | 50:R4:37:SER:N     | 2.77                     | 0.42              |
| 51:R5:35:GLU:O    | 51:R5:36:CYS:C     | 2.63                     | 0.42              |
| 55:R9:1:MET:HE1   | 55:R9:32:HIS:CD2   | 2.53                     | 0.42              |
| 1:XA:33:A:H2'     | 1:XA:34:C:C6       | 2.53                     | 0.42              |
| 1:XA:186:C:H4'    | 20:XT:82:SER:HB3   | 2.01                     | 0.42              |
| 1:XA:372:C:H42    | 1:XA:389:A:H62     | 1.66                     | 0.42              |
| 1:XA:372:C:HO2'   | 1:XA:373:A:P       | 2.42                     | 0.42              |
| 1:XA:598:U:H4'    | 8:XH:94:TYR:CD2    | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:688:G:H2'    | 1:XA:689:C:H6     | 1.83                     | 0.42              |
| 1:XA:1370:G:O3'   | 9:XI:12:GLU:HG3   | 2.19                     | 0.42              |
| 4:XD:36:ARG:HA    | 4:XD:37:PRO:HD2   | 1.82                     | 0.42              |
| 4:XD:146:ILE:H    | 4:XD:146:ILE:CD1  | 2.30                     | 0.42              |
| 6:XF:36:ARG:CZ    | 6:XF:38:GLU:HG2   | 2.50                     | 0.42              |
| 9:XI:8:GLY:CA     | 9:XI:79:LEU:HD12  | 2.49                     | 0.42              |
| 9:XI:88:TYR:O     | 9:XI:89:ASN:HB2   | 2.19                     | 0.42              |
| 15:XO:8:LYS:NZ    | 15:XO:31:LEU:HD11 | 2.34                     | 0.42              |
| 15:XO:10:LYS:O    | 15:XO:14:GLU:HB2  | 2.18                     | 0.42              |
| 16:XP:23:ASP:O    | 16:XP:26:ARG:HB2  | 2.18                     | 0.42              |
| 17:XQ:78:GLU:O    | 17:XQ:79:SER:C    | 2.61                     | 0.42              |
| 18:XR:21:LYS:O    | 18:XR:22:VAL:C    | 2.63                     | 0.42              |
| 19:XS:5:LEU:CD2   | 50:Y4:66:SER:HB2  | 2.47                     | 0.42              |
| 20:XT:13:LEU:CD1  | 20:XT:17:ARG:NH1  | 2.82                     | 0.42              |
| 25:YA:120:U:C2    | 25:YA:149:A:C6    | 3.07                     | 0.42              |
| 25:YA:188:G:H1    | 25:YA:208:C:H42   | 1.67                     | 0.42              |
| 25:YA:952:G:OP1   | 36:YQ:16:ARG:NH1  | 2.35                     | 0.42              |
| 25:YA:1061:U:H4'  | 25:YA:1070:A:H1'  | 2.01                     | 0.42              |
| 25:YA:1153:C:H2'  | 25:YA:1154:G:O4'  | 2.20                     | 0.42              |
| 25:YA:1359:A:N6   | 25:YA:1372:U:C4   | 2.86                     | 0.42              |
| 25:YA:1651:G:N2   | 25:YA:2007:C:C2   | 2.87                     | 0.42              |
| 25:YA:2283:C:OP2  | 52:Y6:5:VAL:HG13  | 2.18                     | 0.42              |
| 27:YD:33:LEU:O    | 27:YD:35:LYS:N    | 2.52                     | 0.42              |
| 30:YG:16:ARG:NE   | 30:YG:31:VAL:HG11 | 2.34                     | 0.42              |
| 30:YG:83:ARG:CB   | 30:YG:86:MET:HE3  | 2.49                     | 0.42              |
| 30:YG:83:ARG:CG   | 30:YG:86:MET:HE3  | 2.49                     | 0.42              |
| 30:YG:121:ASN:HA  | 30:YG:181:ARG:NH2 | 2.34                     | 0.42              |
| 32:YI:29:TYR:C    | 32:YI:32:PRO:HD2  | 2.44                     | 0.42              |
| 34:YO:1:MET:HG2   | 34:YO:67:LYS:HG2  | 2.01                     | 0.42              |
| 35:YP:26:GLY:C    | 35:YP:28:GLY:N    | 2.77                     | 0.42              |
| 36:YQ:20:ALA:C    | 36:YQ:21:THR:HG23 | 2.43                     | 0.42              |
| 36:YQ:20:ALA:HA   | 36:YQ:98:LYS:HB3  | 2.02                     | 0.42              |
| 38:YS:42:ASP:C    | 38:YS:44:LYS:N    | 2.72                     | 0.42              |
| 39:YT:110:ILE:CG2 | 39:YT:111:ARG:N   | 2.82                     | 0.42              |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:CG2  | 2.32                     | 0.42              |
| 47:Y1:72:GLU:O    | 47:Y1:75:GLU:HB2  | 2.19                     | 0.42              |
| 1:QA:113:G:N3     | 1:QA:353:A:O2'    | 2.47                     | 0.42              |
| 1:QA:953:G:H2'    | 1:QA:954:G:O4'    | 2.19                     | 0.42              |
| 1:QA:960:U:H1'    | 1:QA:1223:C:H5'   | 2.01                     | 0.42              |
| 4:QD:127:THR:HG23 | 4:QD:130:GLY:O    | 2.20                     | 0.42              |
| 5:QE:71:LEU:HD11  | 5:QE:113:ALA:O    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:QE:123:LEU:O     | 5:QE:124:GLY:C     | 2.62                     | 0.42              |
| 6:QF:45:LEU:O      | 6:QF:46:ARG:HB2    | 2.19                     | 0.42              |
| 7:QG:79:ARG:NH1    | 7:QG:82:GLY:HA2    | 2.35                     | 0.42              |
| 9:QI:71:SER:O      | 9:QI:74:ILE:N      | 2.52                     | 0.42              |
| 17:QQ:77:VAL:O     | 17:QQ:77:VAL:HG12  | 2.20                     | 0.42              |
| 25:RA:307:G:H22    | 25:RA:310:A:P      | 2.42                     | 0.42              |
| 25:RA:445:C:H5''   | 40:RU:3:ARG:HB2    | 2.00                     | 0.42              |
| 25:RA:851:U:O2'    | 49:R3:45:GLY:HA3   | 2.20                     | 0.42              |
| 25:RA:1268:A:H2'   | 25:RA:1269:A:O4'   | 2.20                     | 0.42              |
| 25:RA:1535:U:N3    | 25:RA:1537:C:H1'   | 2.35                     | 0.42              |
| 25:RA:1893:C:H2'   | 25:RA:1894:C:O4'   | 2.19                     | 0.42              |
| 27:RD:14:ARG:CG    | 27:RD:15:PHE:N     | 2.83                     | 0.42              |
| 27:RD:43:ARG:CZ    | 27:RD:49:ILE:HG21  | 2.49                     | 0.42              |
| 28:RE:3:GLY:HA3    | 28:RE:81:ILE:CD1   | 2.48                     | 0.42              |
| 28:RE:24:THR:HB    | 28:RE:184:VAL:HG23 | 2.01                     | 0.42              |
| 28:RE:35:GLN:HB3   | 28:RE:48:GLN:HB2   | 2.01                     | 0.42              |
| 29:RF:105:VAL:O    | 29:RF:106:ARG:C    | 2.63                     | 0.42              |
| 30:RG:83:ARG:CB    | 30:RG:86:MET:HE3   | 2.49                     | 0.42              |
| 31:RH:58:GLU:O     | 31:RH:60:ARG:N     | 2.53                     | 0.42              |
| 31:RH:120:GLY:O    | 31:RH:136:ILE:HD12 | 2.19                     | 0.42              |
| 32:RI:113:ARG:HG3  | 32:RI:131:LYS:NZ   | 2.34                     | 0.42              |
| 33:RN:26:LEU:HG    | 33:RN:30:ILE:CD1   | 2.49                     | 0.42              |
| 33:RN:42:TRP:HA    | 33:RN:48:MET:CE    | 2.42                     | 0.42              |
| 37:RR:29:LEU:HD11  | 37:RR:48:VAL:CG1   | 2.50                     | 0.42              |
| 40:RU:92:ARG:NH2   | 41:RV:11:GLN:O     | 2.53                     | 0.42              |
| 1:XA:262:A:C6      | 1:XA:263:A:C6      | 3.07                     | 0.42              |
| 1:XA:867:G:O2'     | 1:XA:873:A:N1      | 2.50                     | 0.42              |
| 1:XA:1100:C:OP2    | 2:XB:96:ARG:HG2    | 2.20                     | 0.42              |
| 1:XA:1459:C:OP1    | 20:XT:27:LYS:NZ    | 2.52                     | 0.42              |
| 2:XB:163:PHE:CD2   | 2:XB:185:ILE:HD12  | 2.54                     | 0.42              |
| 2:XB:221:LEU:HD13  | 2:XB:221:LEU:C     | 2.43                     | 0.42              |
| 5:XE:71:LEU:HD11   | 5:XE:113:ALA:O     | 2.19                     | 0.42              |
| 9:XI:71:SER:O      | 9:XI:74:ILE:N      | 2.52                     | 0.42              |
| 15:XO:50:HIS:O     | 15:XO:51:HIS:C     | 2.61                     | 0.42              |
| 18:XR:43:PHE:HA    | 18:XR:51:LEU:HD12  | 2.01                     | 0.42              |
| 19:XS:12:ASP:CG    | 19:XS:37:ARG:HD2   | 2.43                     | 0.42              |
| 19:XS:41:VAL:HG12  | 19:XS:45:VAL:H     | 1.85                     | 0.42              |
| 19:XS:62:ILE:HG22  | 19:XS:63:THR:N     | 2.34                     | 0.42              |
| 19:XS:66:MET:O     | 19:XS:66:MET:HG3   | 2.19                     | 0.42              |
| 25:YA:99:U:H4'     | 25:YA:101:G:C5'    | 2.48                     | 0.42              |
| 25:YA:363(A):A:H2' | 25:YA:363(B):G:C8  | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:851:U:H1'    | 49:Y3:46:ASN:HD21  | 1.84                     | 0.42              |
| 25:YA:2298:A:H2'   | 25:YA:2299:G:O4'   | 2.19                     | 0.42              |
| 25:YA:2784:C:H5''  | 28:YE:41:LYS:NZ    | 2.34                     | 0.42              |
| 28:YE:70:ALA:O     | 28:YE:71:GLY:C     | 2.62                     | 0.42              |
| 28:YE:117:MET:HA   | 28:YE:122:PHE:N    | 2.35                     | 0.42              |
| 28:YE:197:ILE:CD1  | 28:YE:199:ARG:HH12 | 2.26                     | 0.42              |
| 29:YF:128:ALA:O    | 29:YF:129:PHE:CB   | 2.67                     | 0.42              |
| 30:YG:4:ASP:O      | 30:YG:5:VAL:HB     | 2.19                     | 0.42              |
| 30:YG:73:ALA:O     | 30:YG:84:LYS:O     | 2.38                     | 0.42              |
| 30:YG:77:ILE:H     | 30:YG:82:LEU:HB2   | 1.85                     | 0.42              |
| 30:YG:110:ALA:O    | 30:YG:111:LEU:C    | 2.62                     | 0.42              |
| 30:YG:114:ILE:HG22 | 30:YG:117:PHE:HB2  | 2.01                     | 0.42              |
| 32:YI:69:LYS:HG3   | 32:YI:136:VAL:HB   | 2.00                     | 0.42              |
| 32:YI:129:THR:HA   | 32:YI:137:PRO:HA   | 2.01                     | 0.42              |
| 33:YN:43:THR:HA    | 33:YN:44:PRO:HD2   | 1.92                     | 0.42              |
| 35:YP:52:GLU:OE2   | 35:YP:58:THR:N     | 2.52                     | 0.42              |
| 35:YP:64:LYS:HG3   | 54:Y8:25:MET:CE    | 2.50                     | 0.42              |
| 35:YP:65:ARG:C     | 35:YP:66:GLY:O     | 2.59                     | 0.42              |
| 39:YT:96:ARG:HB2   | 39:YT:96:ARG:CZ    | 2.49                     | 0.42              |
| 40:YU:91:ASP:OD2   | 40:YU:96:ALA:HB2   | 2.19                     | 0.42              |
| 40:YU:113:ALA:C    | 40:YU:115:ALA:H    | 2.28                     | 0.42              |
| 45:YZ:26:GLY:HA2   | 45:YZ:85:HIS:CD2   | 2.54                     | 0.42              |
| 51:Y5:20:ARG:HA    | 51:Y5:23:HIS:CE1   | 2.54                     | 0.42              |
| 53:Y7:12:ARG:HH21  | 53:Y7:44:PRO:HB3   | 1.84                     | 0.42              |
| 1:QA:392:G:H2'     | 1:QA:393:A:H8      | 1.85                     | 0.42              |
| 1:QA:518:C:H2'     | 1:QA:530:G:N3      | 2.34                     | 0.42              |
| 1:QA:833:U:H2'     | 1:QA:834:C:H6      | 1.85                     | 0.42              |
| 1:QA:983:A:N1      | 1:QA:1222:G:N2     | 2.66                     | 0.42              |
| 1:QA:1004:A:H2     | 1:QA:1024:G:C8     | 2.37                     | 0.42              |
| 1:QA:1006:C:H2'    | 1:QA:1007:C:C6     | 2.54                     | 0.42              |
| 3:QC:47:LEU:HD11   | 3:QC:76:VAL:CG1    | 2.42                     | 0.42              |
| 3:QC:142:MET:HG2   | 3:QC:149:ALA:HB2   | 2.01                     | 0.42              |
| 4:QD:33:MET:HE2    | 4:QD:37:PRO:HA     | 2.00                     | 0.42              |
| 4:QD:150:GLU:O     | 4:QD:152:SER:N     | 2.53                     | 0.42              |
| 8:QH:33:GLU:O      | 8:QH:36:LEU:N      | 2.53                     | 0.42              |
| 8:QH:109:ILE:HD11  | 8:QH:120:THR:HG22  | 2.01                     | 0.42              |
| 13:QM:54:VAL:O     | 13:QM:58:GLU:OE2   | 2.37                     | 0.42              |
| 15:QO:18:PHE:O     | 15:QO:19:PRO:C     | 2.62                     | 0.42              |
| 18:QR:63:GLN:O     | 18:QR:66:LEU:HB3   | 2.18                     | 0.42              |
| 19:QS:41:VAL:CG1   | 19:QS:45:VAL:H     | 2.32                     | 0.42              |
| 21:QU:2:GLY:C      | 21:QU:4:GLY:N      | 2.78                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:234:C:H2'   | 25:RA:235:U:C6     | 2.53                     | 0.42              |
| 25:RA:530:G:HO2'  | 25:RA:2021:C:HO2'  | 1.60                     | 0.42              |
| 25:RA:832:G:P     | 35:RP:38:GLN:HB3   | 2.60                     | 0.42              |
| 25:RA:924:C:H2'   | 25:RA:925:C:C6     | 2.54                     | 0.42              |
| 25:RA:1007:C:H5'' | 33:RN:35:ARG:NH1   | 2.35                     | 0.42              |
| 25:RA:1061:U:H3'  | 25:RA:1062:G:H5''  | 2.01                     | 0.42              |
| 25:RA:1497:U:H5'' | 25:RA:1498:C:H5    | 1.85                     | 0.42              |
| 25:RA:1860:G:H1   | 25:RA:1882:C:H42   | 1.67                     | 0.42              |
| 25:RA:2154:G:H2'  | 25:RA:2155:G:H8    | 1.82                     | 0.42              |
| 25:RA:2293:C:H2'  | 25:RA:2294:C:H6    | 1.84                     | 0.42              |
| 28:RE:28:ALA:HB3  | 28:RE:93:VAL:CG2   | 2.46                     | 0.42              |
| 28:RE:104:VAL:CG1 | 28:RE:188:VAL:HG23 | 2.49                     | 0.42              |
| 29:RF:179:GLU:CD  | 29:RF:179:GLU:N    | 2.77                     | 0.42              |
| 30:RG:27:ASN:HB3  | 30:RG:30:GLU:OE2   | 2.20                     | 0.42              |
| 30:RG:55:LYS:O    | 30:RG:59:GLU:HB2   | 2.19                     | 0.42              |
| 30:RG:121:ASN:HA  | 30:RG:181:ARG:NH2  | 2.34                     | 0.42              |
| 30:RG:139:LEU:C   | 30:RG:139:LEU:HD12 | 2.44                     | 0.42              |
| 31:RH:89:ILE:CD1  | 31:RH:89:ILE:H     | 2.32                     | 0.42              |
| 31:RH:136:ILE:O   | 31:RH:137:ASP:O    | 2.38                     | 0.42              |
| 39:RT:80:SER:HA   | 39:RT:81:PRO:HD3   | 1.73                     | 0.42              |
| 40:RU:79:PHE:CD2  | 40:RU:83:LEU:HD13  | 2.54                     | 0.42              |
| 40:RU:91:ASP:OD2  | 40:RU:96:ALA:HB2   | 2.19                     | 0.42              |
| 46:R0:72:ARG:HB3  | 46:R0:75:LEU:HB2   | 2.01                     | 0.42              |
| 49:R3:46:ASN:O    | 49:R3:50:VAL:HG22  | 2.20                     | 0.42              |
| 50:R4:54:GLY:HA2  | 50:R4:57:GLU:CG    | 2.50                     | 0.42              |
| 51:R5:20:ARG:HA   | 51:R5:23:HIS:CE1   | 2.54                     | 0.42              |
| 1:XA:22:G:H4'     | 1:XA:885:G:C8      | 2.54                     | 0.42              |
| 1:XA:1054:C:N4    | 23:XY:34:C:C6      | 2.88                     | 0.42              |
| 1:XA:1301:U:O2    | 1:XA:1301:U:H2'    | 2.19                     | 0.42              |
| 1:XA:1352:C:H42   | 1:XA:1370:G:H1     | 1.67                     | 0.42              |
| 1:XA:1451:A:N3    | 1:XA:1451:A:H2'    | 2.33                     | 0.42              |
| 2:XB:200:ILE:HD12 | 2:XB:200:ILE:N     | 2.34                     | 0.42              |
| 4:XD:206:PHE:CD2  | 4:XD:207:TYR:HD1   | 2.37                     | 0.42              |
| 5:XE:56:GLN:C     | 5:XE:58:ALA:H      | 2.26                     | 0.42              |
| 7:XG:11:GLN:HG3   | 7:XG:12:LEU:H      | 1.85                     | 0.42              |
| 7:XG:140:ASP:O    | 7:XG:142:GLU:N     | 2.52                     | 0.42              |
| 8:XH:11:THR:HA    | 8:XH:14:ARG:NH1    | 2.34                     | 0.42              |
| 8:XH:85:ARG:HA    | 8:XH:135:CYS:HB3   | 2.02                     | 0.42              |
| 10:XJ:49:VAL:HG13 | 10:XJ:50:ILE:N     | 2.34                     | 0.42              |
| 13:XM:88:ARG:HD2  | 13:XM:88:ARG:O     | 2.19                     | 0.42              |
| 14:XN:9:LYS:HG2   | 14:XN:9:LYS:O      | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:YN:48:ALA:HA    | 14:YN:53:LEU:HD12  | 2.02                     | 0.42              |
| 16:XP:83:GLU:HG3   | 16:XP:84:ALA:N     | 2.33                     | 0.42              |
| 18:XR:74:ARG:NH2   | 18:XR:81:PHE:HA    | 2.35                     | 0.42              |
| 19:XS:21:GLU:HG3   | 19:XS:22:LEU:CD1   | 2.49                     | 0.42              |
| 19:XS:30:LEU:C     | 19:XS:30:LEU:HD22  | 2.45                     | 0.42              |
| 25:YA:389:G:O6     | 35:YP:70:GLN:HB3   | 2.20                     | 0.42              |
| 25:YA:568:U:N3     | 25:YA:571:A:OP2    | 2.34                     | 0.42              |
| 25:YA:1071:G:H8    | 25:YA:1071:G:O5'   | 2.02                     | 0.42              |
| 25:YA:1155:A:O3'   | 40:YU:55:ARG:NH1   | 2.50                     | 0.42              |
| 25:YA:1484:G:H1    | 25:YA:1505:C:N4    | 2.14                     | 0.42              |
| 25:YA:1716:U:O2'   | 25:YA:1717:G:H5'   | 2.20                     | 0.42              |
| 25:YA:2605:U:H2'   | 25:YA:2606:C:C6    | 2.55                     | 0.42              |
| 25:YA:2875:C:C4'   | 39:YT:5:ALA:HB2    | 2.49                     | 0.42              |
| 27:YD:71:ASP:CB    | 27:YD:103:ARG:HH22 | 2.32                     | 0.42              |
| 27:YD:108:PRO:HG2  | 27:YD:111:LEU:HB2  | 2.01                     | 0.42              |
| 27:YD:158:ALA:HB3  | 27:YD:161:THR:CG2  | 2.49                     | 0.42              |
| 28:YE:104:VAL:CG1  | 28:YE:188:VAL:HG23 | 2.49                     | 0.42              |
| 28:YE:176:ILE:HD12 | 28:YE:176:ILE:N    | 2.35                     | 0.42              |
| 29:YF:11:VAL:HG12  | 29:YF:12:LEU:H     | 1.84                     | 0.42              |
| 29:YF:32:LEU:C     | 29:YF:32:LEU:CD1   | 2.83                     | 0.42              |
| 30:YG:117:PHE:CE1  | 30:YG:119:GLY:CA   | 3.03                     | 0.42              |
| 31:YH:58:GLU:O     | 31:YH:60:ARG:N     | 2.52                     | 0.42              |
| 31:YH:136:ILE:O    | 31:YH:137:ASP:O    | 2.38                     | 0.42              |
| 32:YI:9:LEU:O      | 32:YI:10:GLU:HG3   | 2.19                     | 0.42              |
| 34:YO:61:VAL:O     | 34:YO:61:VAL:HG13  | 2.18                     | 0.42              |
| 35:YP:119:GLU:HA   | 35:YP:119:GLU:OE1  | 2.18                     | 0.42              |
| 38:YS:15:ARG:O     | 38:YS:19:LYS:HD3   | 2.20                     | 0.42              |
| 41:YV:38:LEU:CD1   | 41:YV:55:ALA:HB1   | 2.50                     | 0.42              |
| 41:YV:59:ALA:HA    | 41:YV:95:LEU:O     | 2.19                     | 0.42              |
| 44:YY:95:LYS:HA    | 44:YY:101:LYS:N    | 2.33                     | 0.42              |
| 48:Y2:16:LEU:C     | 48:Y2:16:LEU:HD12  | 2.44                     | 0.42              |
| 48:Y2:27:GLU:N     | 48:Y2:27:GLU:CD    | 2.77                     | 0.42              |
| 52:Y6:50:ARG:HH11  | 52:Y6:50:ARG:HG2   | 1.84                     | 0.42              |
| 54:Y8:28:GLY:O     | 54:Y8:29:LYS:O     | 2.36                     | 0.42              |
| 1:QA:573:A:N3      | 1:QA:883:C:O2'     | 2.53                     | 0.42              |
| 1:QA:1086:U:H3     | 1:QA:1099:G:H22    | 1.66                     | 0.42              |
| 2:QB:83:MET:C      | 2:QB:85:ALA:H      | 2.27                     | 0.42              |
| 3:QC:35:GLU:O      | 3:QC:38:ARG:N      | 2.53                     | 0.42              |
| 3:QC:58:GLU:HB2    | 3:QC:65:ALA:HB3    | 2.01                     | 0.42              |
| 3:QC:88:ARG:NH2    | 3:QC:101:LEU:O     | 2.53                     | 0.42              |
| 4:QD:13:ARG:HB3    | 4:QD:33:MET:HE3    | 1.92                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:59:ARG:HA     | 4:QD:59:ARG:NE     | 2.34                     | 0.42              |
| 5:QE:56:GLN:C      | 5:QE:58:ALA:N      | 2.78                     | 0.42              |
| 8:QH:95:VAL:O      | 8:QH:95:VAL:HG23   | 2.20                     | 0.42              |
| 9:QI:25:LYS:O      | 9:QI:60:ASP:OD1    | 2.37                     | 0.42              |
| 11:QK:62:GLN:C     | 11:QK:64:ALA:N     | 2.76                     | 0.42              |
| 13:QM:13:LYS:HA    | 13:QM:44:ARG:CD    | 2.48                     | 0.42              |
| 13:QM:119:GLY:O    | 13:QM:120:LYS:C    | 2.63                     | 0.42              |
| 15:QO:58:MET:O     | 15:QO:59:MET:C     | 2.61                     | 0.42              |
| 16:QP:1:MET:O      | 16:QP:2:VAL:C      | 2.63                     | 0.42              |
| 18:QR:76:LEU:HD22  | 18:QR:76:LEU:N     | 2.35                     | 0.42              |
| 20:QT:36:LEU:HD13  | 20:QT:36:LEU:HA    | 1.82                     | 0.42              |
| 25:RA:1162:G:H1'   | 41:RV:23:GLU:OE2   | 2.19                     | 0.42              |
| 25:RA:1923:U:H2'   | 25:RA:1924:C:C6    | 2.54                     | 0.42              |
| 25:RA:2636:U:OP1   | 28:RE:79:ARG:HG3   | 2.19                     | 0.42              |
| 25:RA:2712:U:O2'   | 25:RA:2712(A):A:H8 | 2.03                     | 0.42              |
| 27:RD:33:LEU:HB3   | 27:RD:34:VAL:H     | 1.48                     | 0.42              |
| 27:RD:182:LEU:N    | 27:RD:272:ALA:HB3  | 2.32                     | 0.42              |
| 28:RE:72:VAL:O     | 28:RE:73:GLU:C     | 2.63                     | 0.42              |
| 28:RE:143:ASN:HB2  | 28:RE:147:PRO:HD2  | 2.00                     | 0.42              |
| 29:RF:164:ARG:HG2  | 29:RF:164:ARG:NH1  | 2.34                     | 0.42              |
| 31:RH:26:VAL:CG1   | 31:RH:33:LEU:HB2   | 2.50                     | 0.42              |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CD   | 2.49                     | 0.42              |
| 32:RI:21:VAL:HG21  | 32:RI:25:TYR:HD1   | 1.83                     | 0.42              |
| 33:RN:75:TYR:HA    | 33:RN:82:LEU:HA    | 2.01                     | 0.42              |
| 34:RO:104:ARG:C    | 34:RO:106:LEU:N    | 2.77                     | 0.42              |
| 35:RP:115:LEU:HB3  | 35:RP:131:SER:HB2  | 2.02                     | 0.42              |
| 35:RP:119:GLU:OE1  | 35:RP:119:GLU:HA   | 2.19                     | 0.42              |
| 38:RS:88:ASP:CG    | 38:RS:89:ARG:N     | 2.77                     | 0.42              |
| 40:RU:104:GLN:H    | 40:RU:104:GLN:CD   | 2.16                     | 0.42              |
| 40:RU:113:ALA:C    | 40:RU:115:ALA:H    | 2.27                     | 0.42              |
| 42:RW:71:VAL:HA    | 42:RW:107:LEU:HD12 | 2.02                     | 0.42              |
| 44:RY:75:ILE:C     | 44:RY:75:ILE:CD1   | 2.92                     | 0.42              |
| 45:RZ:111:VAL:HG13 | 45:RZ:112:ARG:N    | 2.34                     | 0.42              |
| 47:R1:66:HIS:C     | 47:R1:68:PRO:CD    | 2.92                     | 0.42              |
| 47:R1:72:GLU:O     | 47:R1:75:GLU:HB2   | 2.20                     | 0.42              |
| 48:R2:16:LEU:C     | 48:R2:16:LEU:HD12  | 2.45                     | 0.42              |
| 49:R3:37:LEU:HD12  | 49:R3:43:ILE:CG2   | 2.50                     | 0.42              |
| 1:XA:409:G:H3'     | 1:XA:410:G:H8      | 1.84                     | 0.42              |
| 1:XA:741:G:H2'     | 1:XA:742:G:O4'     | 2.18                     | 0.42              |
| 1:XA:1483:A:H2     | 25:YA:1959:G:N3    | 2.18                     | 0.42              |
| 2:XB:16:HIS:CD2    | 2:XB:213:LEU:HD13  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:XB:178:ARG:CD   | 8:XH:71:GLY:C     | 2.93                     | 0.42              |
| 5:XE:128:PRO:O    | 5:XE:129:ILE:C    | 2.63                     | 0.42              |
| 6:XF:46:ARG:HG3   | 6:XF:47:ARG:N     | 2.34                     | 0.42              |
| 7:XG:15:ASP:OD1   | 7:XG:23:VAL:HG11  | 2.19                     | 0.42              |
| 13:XM:19:LEU:HD22 | 13:XM:19:LEU:N    | 2.33                     | 0.42              |
| 14:YN:6:LEU:HD23  | 14:YN:6:LEU:C     | 2.45                     | 0.42              |
| 15:XO:64:ARG:CD   | 15:XO:68:ARG:NH2  | 2.82                     | 0.42              |
| 18:XR:29:PHE:N    | 18:XR:29:PHE:HD2  | 2.17                     | 0.42              |
| 19:XS:29:ARG:HD3  | 19:XS:30:LEU:H    | 1.84                     | 0.42              |
| 19:XS:41:VAL:CG1  | 19:XS:45:VAL:H    | 2.32                     | 0.42              |
| 20:XT:14:LYS:O    | 20:XT:15:ARG:C    | 2.62                     | 0.42              |
| 20:XT:81:LYS:C    | 20:XT:83:ARG:H    | 2.28                     | 0.42              |
| 21:XU:5:ASP:O     | 21:XU:11:GLY:HA3  | 2.20                     | 0.42              |
| 22:XV:15:G:N2     | 22:XV:48:C:H42    | 2.17                     | 0.42              |
| 25:YA:184:C:H2'   | 25:YA:185:U:H6    | 1.82                     | 0.42              |
| 25:YA:451:C:H4'   | 29:YF:52:LYS:HZ1  | 1.80                     | 0.42              |
| 25:YA:994:C:OP1   | 40:YU:53:ARG:NH2  | 2.52                     | 0.42              |
| 27:YD:2:ALA:O     | 27:YD:3:VAL:CB    | 2.68                     | 0.42              |
| 27:YD:75:ILE:HG21 | 27:YD:99:ASP:HB2  | 2.02                     | 0.42              |
| 28:YE:7:VAL:HG11  | 39:YT:1:MET:HE3   | 2.00                     | 0.42              |
| 28:YE:72:VAL:O    | 28:YE:73:GLU:C    | 2.62                     | 0.42              |
| 31:YH:26:VAL:CG1  | 31:YH:33:LEU:HB2  | 2.50                     | 0.42              |
| 31:YH:89:ILE:CD1  | 31:YH:89:ILE:H    | 2.32                     | 0.42              |
| 35:YP:47:ASP:CG   | 35:YP:49:ARG:NH1  | 2.77                     | 0.42              |
| 35:YP:114:ILE:CD1 | 35:YP:130:PHE:CE1 | 2.98                     | 0.42              |
| 36:YQ:27:VAL:HG11 | 36:YQ:134:ARG:HG3 | 2.00                     | 0.42              |
| 40:YU:79:PHE:CD2  | 40:YU:83:LEU:HD13 | 2.54                     | 0.42              |
| 44:YY:20:TYR:C    | 44:YY:21:LYS:O    | 2.62                     | 0.42              |
| 47:Y1:29:GLY:C    | 47:Y1:31:GLY:H    | 2.27                     | 0.42              |
| 50:Y4:12:ALA:HB1  | 50:Y4:30:GLU:N    | 2.35                     | 0.42              |
| 50:Y4:54:GLY:HA2  | 50:Y4:57:GLU:CG   | 2.50                     | 0.42              |
| 52:Y6:25:LYS:HE2  | 52:Y6:27:LYS:CD   | 2.49                     | 0.42              |
| 52:Y6:36:LEU:HD13 | 52:Y6:50:ARG:HH12 | 1.81                     | 0.42              |
| 1:QA:652:U:O4     | 1:QA:752:G:H2'    | 2.19                     | 0.42              |
| 1:QA:939:G:H5''   | 7:QG:102:ARG:CZ   | 2.50                     | 0.42              |
| 1:QA:1226:C:N4    | 13:QM:104:ARG:HD2 | 2.34                     | 0.42              |
| 1:QA:1328:C:OP1   | 21:QU:21:TYR:OH   | 2.29                     | 0.42              |
| 1:QA:1446:A:HO2'  | 1:QA:1447:G:P     | 2.41                     | 0.42              |
| 2:QB:69:LEU:HD12  | 2:QB:91:PRO:O     | 2.19                     | 0.42              |
| 2:QB:130:ARG:NH2  | 2:QB:138:LEU:HD21 | 2.34                     | 0.42              |
| 2:QB:197:VAL:CG1  | 2:QB:198:ASP:N    | 2.82                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:91:SER:O      | 4:QD:92:VAL:C      | 2.62                     | 0.42              |
| 4:QD:93:PHE:CE1    | 4:QD:97:LEU:HD11   | 2.55                     | 0.42              |
| 7:QG:18:TYR:CD2    | 7:QG:59:LEU:HD13   | 2.55                     | 0.42              |
| 7:QG:150:ALA:HA    | 11:QK:59:TYR:CD2   | 2.55                     | 0.42              |
| 8:QH:26:VAL:O      | 8:QH:27:PRO:C      | 2.63                     | 0.42              |
| 8:QH:86:ILE:CB     | 8:QH:133:LEU:HD22  | 2.49                     | 0.42              |
| 9:QI:85:LEU:HD12   | 9:QI:85:LEU:C      | 2.45                     | 0.42              |
| 19:QS:7:LYS:CG     | 19:QS:8:GLY:N      | 2.83                     | 0.42              |
| 19:QS:30:LEU:O     | 19:QS:31:ILE:HB    | 2.19                     | 0.42              |
| 20:QT:96:GLY:O     | 20:QT:99:LEU:CD1   | 2.67                     | 0.42              |
| 25:RA:380:U:O3'    | 47:R1:16:ASN:HB2   | 2.20                     | 0.42              |
| 25:RA:565:C:H4'    | 25:RA:1253:A:C6    | 2.55                     | 0.42              |
| 25:RA:1042:G:H2'   | 25:RA:1043:C:C6    | 2.55                     | 0.42              |
| 25:RA:1228:G:OP1   | 40:RU:13:LYS:HG2   | 2.20                     | 0.42              |
| 25:RA:1365:A:OP2   | 47:R1:3:LYS:HB2    | 2.19                     | 0.42              |
| 25:RA:2316:C:H2'   | 25:RA:2317:C:C6    | 2.54                     | 0.42              |
| 25:RA:2405:G:O2'   | 25:RA:2406:U:OP2   | 2.33                     | 0.42              |
| 30:RG:63:ILE:HG12  | 30:RG:64:THR:N     | 2.33                     | 0.42              |
| 31:RH:27:LYS:HD2   | 31:RH:27:LYS:C     | 2.44                     | 0.42              |
| 33:RN:43:THR:HA    | 33:RN:44:PRO:HD2   | 1.92                     | 0.42              |
| 34:RO:1:MET:HG2    | 34:RO:67:LYS:HG2   | 2.01                     | 0.42              |
| 34:RO:97:ARG:CA    | 34:RO:117:LEU:HD22 | 2.50                     | 0.42              |
| 35:RP:26:GLY:C     | 35:RP:28:GLY:N     | 2.78                     | 0.42              |
| 36:RQ:27:VAL:HG11  | 36:RQ:134:ARG:HG3  | 2.00                     | 0.42              |
| 36:RQ:118:LEU:HD23 | 36:RQ:118:LEU:HA   | 1.87                     | 0.42              |
| 36:RQ:139:GLU:H    | 36:RQ:139:GLU:CD   | 2.28                     | 0.42              |
| 37:RR:55:ALA:HA    | 37:RR:80:PHE:CE2   | 2.55                     | 0.42              |
| 39:RT:110:ILE:CG2  | 39:RT:111:ARG:N    | 2.82                     | 0.42              |
| 39:RT:134:GLU:OE1  | 39:RT:135:ALA:N    | 2.53                     | 0.42              |
| 44:RY:60:PHE:CD2   | 44:RY:60:PHE:N     | 2.87                     | 0.42              |
| 47:R1:74:VAL:O     | 47:R1:74:VAL:CG1   | 2.64                     | 0.42              |
| 50:R4:6:HIS:O      | 50:R4:7:PRO:C      | 2.63                     | 0.42              |
| 1:XA:1366:C:H2'    | 1:XA:1367:C:H6     | 1.85                     | 0.42              |
| 1:XA:1446:A:O2'    | 1:XA:1447:G:P      | 2.78                     | 0.42              |
| 2:XB:5:ILE:HB      | 2:XB:221:LEU:HD23  | 2.01                     | 0.42              |
| 2:XB:99:GLY:O      | 2:XB:108:ILE:HD11  | 2.19                     | 0.42              |
| 2:XB:239:VAL:O     | 2:XB:240:GLN:C     | 2.62                     | 0.42              |
| 3:XC:23:TYR:CD2    | 3:XC:24:ALA:N      | 2.88                     | 0.42              |
| 3:XC:83:ARG:O      | 3:XC:86:VAL:HG22   | 2.20                     | 0.42              |
| 4:XD:150:GLU:O     | 4:XD:152:SER:N     | 2.53                     | 0.42              |
| 5:XE:31:LEU:HD23   | 5:XE:45:PHE:HD1    | 1.85                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:64:GLN:C      | 7:XG:66:VAL:N      | 2.77                     | 0.42              |
| 7:XG:89:MET:CE     | 7:XG:156:TRP:H     | 2.22                     | 0.42              |
| 7:XG:108:ALA:C     | 7:XG:110:GLN:N     | 2.77                     | 0.42              |
| 9:XI:6:GLY:HA3     | 9:XI:84:ALA:HB2    | 2.01                     | 0.42              |
| 9:XI:35:GLU:O      | 9:XI:35:GLU:HG2    | 2.19                     | 0.42              |
| 9:XI:118:LYS:HZ3   | 9:XI:118:LYS:HB3   | 1.85                     | 0.42              |
| 13:XM:118:ALA:O    | 22:XV:28:C:O3'     | 2.37                     | 0.42              |
| 15:XO:18:PHE:O     | 15:XO:19:PRO:C     | 2.62                     | 0.42              |
| 25:YA:2227:A:H5''  | 27:YD:263:ARG:HH11 | 1.82                     | 0.42              |
| 25:YA:2636:U:OP2   | 28:YE:79:ARG:NH1   | 2.52                     | 0.42              |
| 25:YA:2752:C:H2'   | 25:YA:2753:A:O4'   | 2.19                     | 0.42              |
| 25:YA:2869:G:H2'   | 25:YA:2870:C:O4'   | 2.20                     | 0.42              |
| 27:YD:25:THR:HG23  | 27:YD:27:THR:HB    | 2.02                     | 0.42              |
| 28:YE:25:VAL:CG1   | 39:YT:11:GLU:HG2   | 2.50                     | 0.42              |
| 28:YE:28:ALA:HB3   | 28:YE:93:VAL:CG2   | 2.47                     | 0.42              |
| 28:YE:31:CYS:HB3   | 28:YE:49:LEU:HG    | 2.01                     | 0.42              |
| 28:YE:36:ARG:HB3   | 28:YE:36:ARG:NH1   | 2.30                     | 0.42              |
| 29:YF:62:ARG:NH1   | 29:YF:62:ARG:CB    | 2.82                     | 0.42              |
| 29:YF:123:LEU:HD12 | 29:YF:124:LEU:H    | 1.82                     | 0.42              |
| 30:YG:55:LYS:O     | 30:YG:59:GLU:HB2   | 2.19                     | 0.42              |
| 31:YH:77:LYS:HB3   | 31:YH:77:LYS:HZ2   | 1.78                     | 0.42              |
| 34:YO:20:MET:O     | 34:YO:41:ALA:CB    | 2.67                     | 0.42              |
| 35:YP:115:LEU:HB3  | 35:YP:131:SER:HB2  | 2.02                     | 0.42              |
| 35:YP:135:LEU:HD13 | 35:YP:139:LYS:HE3  | 2.01                     | 0.42              |
| 36:YQ:51:ARG:O     | 36:YQ:52:VAL:C     | 2.63                     | 0.42              |
| 38:YS:52:SER:HB2   | 38:YS:55:ALA:CB    | 2.49                     | 0.42              |
| 39:YT:6:LEU:HD12   | 39:YT:9:LEU:HD12   | 2.01                     | 0.42              |
| 44:YY:91:GLU:CG    | 44:YY:92:ASN:N     | 2.83                     | 0.42              |
| 47:Y1:66:HIS:C     | 47:Y1:68:PRO:CD    | 2.92                     | 0.42              |
| 49:Y3:7:LYS:O      | 49:Y3:7:LYS:HG2    | 2.19                     | 0.42              |
| 52:Y6:24:GLU:HB3   | 52:Y6:25:LYS:H     | 1.56                     | 0.42              |
| 53:Y7:9:ARG:NH1    | 53:Y7:47:ARG:HG3   | 2.35                     | 0.42              |
| 55:Y9:17:ILE:CG2   | 55:Y9:18:ARG:N     | 2.82                     | 0.42              |
| 1:QA:452:A:O2'     | 1:QA:453:A:O5'     | 2.37                     | 0.42              |
| 1:QA:681:C:H2'     | 1:QA:682:G:C8      | 2.55                     | 0.42              |
| 1:QA:813:U:H6      | 1:QA:813:U:O5'     | 2.02                     | 0.42              |
| 2:QB:30:ARG:HH21   | 2:QB:194:PRO:HG2   | 1.82                     | 0.42              |
| 5:QE:31:LEU:HD23   | 5:QE:45:PHE:HD1    | 1.85                     | 0.42              |
| 8:QH:102:ARG:NH1   | 8:QH:105:ARG:CZ    | 2.80                     | 0.42              |
| 9:QI:6:GLY:HA3     | 9:QI:84:ALA:HB2    | 2.01                     | 0.42              |
| 11:QK:21:ILE:HD13  | 11:QK:84:VAL:HG12  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:QK:72:ALA:HB1  | 11:QK:77:MET:HG2   | 2.02                     | 0.42              |
| 12:QL:38:THR:HG22 | 12:QL:57:LYS:HB3   | 2.01                     | 0.42              |
| 17:QQ:27:PHE:HA   | 17:QQ:28:PRO:HD3   | 1.92                     | 0.42              |
| 17:QQ:76:LEU:HD21 | 17:QQ:79:SER:HB2   | 2.01                     | 0.42              |
| 19:QS:15:LEU:N    | 19:QS:15:LEU:CD2   | 2.79                     | 0.42              |
| 19:QS:18:LYS:O    | 19:QS:18:LYS:HD2   | 2.19                     | 0.42              |
| 20:QT:10:LEU:O    | 20:QT:12:ALA:N     | 2.53                     | 0.42              |
| 20:QT:13:LEU:CD1  | 20:QT:17:ARG:NH1   | 2.82                     | 0.42              |
| 21:QU:5:ASP:O     | 21:QU:11:GLY:HA3   | 2.20                     | 0.42              |
| 25:RA:813:U:H2'   | 25:RA:814:C:C6     | 2.55                     | 0.42              |
| 25:RA:1032:A:H4'  | 55:R9:16:VAL:HG11  | 2.01                     | 0.42              |
| 25:RA:1139:G:O2'  | 25:RA:1143:A:N1    | 2.47                     | 0.42              |
| 25:RA:1487:G:H1   | 25:RA:1502:C:H42   | 1.67                     | 0.42              |
| 25:RA:1578:U:C2'  | 25:RA:1579:A:H5'   | 2.49                     | 0.42              |
| 25:RA:2489:G:N2   | 25:RA:2491:U:O4    | 2.44                     | 0.42              |
| 25:RA:2683:C:N3   | 25:RA:2727:G:O2'   | 2.51                     | 0.42              |
| 26:RB:41:U:N3     | 30:RG:70:VAL:HG23  | 2.34                     | 0.42              |
| 27:RD:9:TYR:CZ    | 27:RD:13:ARG:HD3   | 2.54                     | 0.42              |
| 27:RD:158:ALA:HB3 | 27:RD:161:THR:CG2  | 2.49                     | 0.42              |
| 27:RD:165:ILE:O   | 27:RD:166:GLN:NE2  | 2.53                     | 0.42              |
| 27:RD:168:ARG:O   | 27:RD:169:GLU:HB2  | 2.19                     | 0.42              |
| 28:RE:10:GLY:HA3  | 39:RT:8:LYS:HD3    | 2.02                     | 0.42              |
| 28:RE:117:MET:HA  | 28:RE:122:PHE:N    | 2.35                     | 0.42              |
| 28:RE:128:SER:O   | 28:RE:129:HIS:HB2  | 2.19                     | 0.42              |
| 28:RE:137:HIS:CB  | 28:RE:138:PRO:HD2  | 2.42                     | 0.42              |
| 29:RF:63:LYS:HE2  | 29:RF:67:GLN:HB2   | 2.01                     | 0.42              |
| 29:RF:198:ALA:HA  | 29:RF:201:VAL:CG1  | 2.41                     | 0.42              |
| 30:RG:16:ARG:NE   | 30:RG:31:VAL:HG11  | 2.34                     | 0.42              |
| 30:RG:51:ARG:NH1  | 30:RG:51:ARG:CB    | 2.83                     | 0.42              |
| 33:RN:62:VAL:HG12 | 33:RN:66:LYS:HB2   | 2.01                     | 0.42              |
| 38:RS:51:ALA:HB3  | 38:RS:73:LEU:HD23  | 2.01                     | 0.42              |
| 38:RS:83:LYS:HE3  | 38:RS:84:GLN:HG3   | 2.02                     | 0.42              |
| 40:RU:97:ASP:HA   | 40:RU:100:VAL:HG23 | 2.02                     | 0.42              |
| 40:RU:99:ALA:HA   | 40:RU:106:PHE:HB2  | 2.01                     | 0.42              |
| 41:RV:59:ALA:HA   | 41:RV:95:LEU:O     | 2.19                     | 0.42              |
| 44:RY:20:TYR:CE1  | 44:RY:42:VAL:HA    | 2.55                     | 0.42              |
| 45:RZ:129:SER:C   | 45:RZ:131:ARG:H    | 2.27                     | 0.42              |
| 52:R6:19:ARG:HA   | 52:R6:19:ARG:HD2   | 1.76                     | 0.42              |
| 1:XA:135:C:H2'    | 1:XA:136:C:H5'     | 2.01                     | 0.42              |
| 1:XA:253:U:H2'    | 1:XA:254:G:H8      | 1.84                     | 0.42              |
| 1:XA:346:G:H1'    | 1:XA:347:G:H5'     | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:582:U:H2'     | 1:XA:583:A:H8     | 1.84                     | 0.42              |
| 1:XA:1200:C:O2'    | 1:XA:1201:A:OP2   | 2.33                     | 0.42              |
| 1:XA:1285:A:H4'    | 1:XA:1286:A:O5'   | 2.19                     | 0.42              |
| 1:XA:1365:G:H2'    | 1:XA:1366:C:C6    | 2.55                     | 0.42              |
| 2:XB:83:MET:C      | 2:XB:85:ALA:H     | 2.27                     | 0.42              |
| 2:XB:178:ARG:NH2   | 8:XH:68:ARG:HH22  | 2.17                     | 0.42              |
| 3:XC:35:GLU:O      | 3:XC:38:ARG:N     | 2.53                     | 0.42              |
| 4:XD:91:SER:O      | 4:XD:92:VAL:C     | 2.63                     | 0.42              |
| 4:XD:202:LEU:C     | 4:XD:204:ILE:N    | 2.78                     | 0.42              |
| 6:XF:45:LEU:O      | 6:XF:46:ARG:HB2   | 2.19                     | 0.42              |
| 6:XF:88:VAL:HG12   | 6:XF:89:MET:N     | 2.34                     | 0.42              |
| 7:XG:6:ARG:O       | 7:XG:7:ALA:C      | 2.62                     | 0.42              |
| 12:XL:53:ARG:HH12  | 12:XL:92:ASP:CB   | 2.33                     | 0.42              |
| 12:XL:119:LYS:HB2  | 12:XL:120:TYR:HD1 | 1.83                     | 0.42              |
| 13:XM:16:ASP:HB3   | 13:XM:34:LEU:CD1  | 2.49                     | 0.42              |
| 19:XS:4:SER:O      | 19:XS:5:LEU:HD13  | 2.20                     | 0.42              |
| 19:XS:30:LEU:O     | 19:XS:31:ILE:HB   | 2.19                     | 0.42              |
| 20:XT:50:GLU:O     | 20:XT:51:GLU:C    | 2.62                     | 0.42              |
| 20:XT:99:LEU:O     | 20:XT:100:ILE:CB  | 2.68                     | 0.42              |
| 21:XU:2:GLY:C      | 21:XU:4:GLY:N     | 2.78                     | 0.42              |
| 22:XV:43:A:H2'     | 22:XV:44:A:C8     | 2.54                     | 0.42              |
| 25:YA:155:C:H5'    | 25:YA:161:U:OP2   | 2.20                     | 0.42              |
| 25:YA:329:G:OP2    | 44:YY:71:LYS:HE3  | 2.19                     | 0.42              |
| 25:YA:1057:A:H62   | 25:YA:1086:A:H2'  | 1.84                     | 0.42              |
| 25:YA:1093:G:OP1   | 31:YH:170:ARG:HD2 | 2.18                     | 0.42              |
| 25:YA:1429:G:H2'   | 25:YA:1430:C:C6   | 2.54                     | 0.42              |
| 25:YA:2051:A:H5'   | 25:YA:2578:G:O4'  | 2.19                     | 0.42              |
| 25:YA:2544:G:H8    | 25:YA:2544:G:O5'  | 2.03                     | 0.42              |
| 25:YA:2593:U:H2'   | 25:YA:2594:C:C6   | 2.55                     | 0.42              |
| 25:YA:2597:G:H2'   | 25:YA:2598:A:C8   | 2.55                     | 0.42              |
| 28:YE:16:ARG:C     | 28:YE:17:ASP:CG   | 2.86                     | 0.42              |
| 28:YE:35:GLN:HB3   | 28:YE:48:GLN:HB2  | 2.01                     | 0.42              |
| 28:YE:128:SER:O    | 28:YE:129:HIS:HB2 | 2.19                     | 0.42              |
| 28:YE:143:ASN:HB2  | 28:YE:147:PRO:HD2 | 2.01                     | 0.42              |
| 28:YE:152:LYS:HG2  | 33:YN:78:TYR:CD1  | 2.55                     | 0.42              |
| 29:YF:183:VAL:HG22 | 29:YF:184:TYR:N   | 2.35                     | 0.42              |
| 30:YG:99:MET:O     | 30:YG:103:LEU:HB2 | 2.20                     | 0.42              |
| 30:YG:126:ASP:CG   | 30:YG:130:ASN:HB2 | 2.45                     | 0.42              |
| 31:YH:84:SER:O     | 31:YH:85:LYS:CB   | 2.64                     | 0.42              |
| 32:YI:57:ARG:HA    | 32:YI:60:GLU:HB3  | 2.02                     | 0.42              |
| 33:YN:10:GLU:OE2   | 33:YN:11:PRO:CD   | 2.68                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:75:TYR:HA    | 33:YN:82:LEU:HA    | 2.02                     | 0.42              |
| 34:YO:104:ARG:C    | 34:YO:106:LEU:N    | 2.77                     | 0.42              |
| 34:YO:116:SER:C    | 34:YO:118:ALA:N    | 2.76                     | 0.42              |
| 35:YP:83:VAL:HG11  | 35:YP:112:LEU:HD21 | 1.97                     | 0.42              |
| 36:YQ:20:ALA:HB2   | 36:YQ:99:PRO:HD2   | 1.99                     | 0.42              |
| 38:YS:18:ILE:O     | 38:YS:19:LYS:C     | 2.62                     | 0.42              |
| 39:YT:54:ARG:HA    | 39:YT:59:THR:HG23  | 2.02                     | 0.42              |
| 41:YV:25:LEU:H     | 41:YV:92:THR:CG2   | 2.29                     | 0.42              |
| 43:YX:60:ARG:HH12  | 53:Y7:47:ARG:HH22  | 1.67                     | 0.42              |
| 52:Y6:7:ILE:O      | 52:Y6:8:LYS:CG     | 2.68                     | 0.42              |
| 55:Y9:1:MET:HE2    | 55:Y9:10:ILE:CD1   | 2.49                     | 0.42              |
| 1:QA:355:C:C1'     | 1:QA:388:G:H2'     | 2.49                     | 0.42              |
| 1:QA:791:G:H2'     | 1:QA:792:A:H5'     | 2.02                     | 0.42              |
| 1:QA:1315:U:H2'    | 1:QA:1316:G:O4'    | 2.19                     | 0.42              |
| 1:QA:1333:A:C2     | 1:QA:1334:G:H1'    | 2.55                     | 0.42              |
| 1:QA:1402:C:H2'    | 1:QA:1403:C:O4'    | 2.20                     | 0.42              |
| 2:QB:25:ASN:C      | 2:QB:27:LYS:H      | 2.24                     | 0.42              |
| 2:QB:142:LEU:O     | 2:QB:145:LEU:HB2   | 2.19                     | 0.42              |
| 3:QC:120:VAL:O     | 3:QC:123:GLN:HB2   | 2.20                     | 0.42              |
| 4:QD:29:PRO:CG     | 4:QD:30:LYS:CE     | 2.86                     | 0.42              |
| 4:QD:178:VAL:O     | 4:QD:179:GLU:C     | 2.63                     | 0.42              |
| 5:QE:26:PHE:CD1    | 5:QE:26:PHE:N      | 2.87                     | 0.42              |
| 9:QI:35:GLU:HG2    | 9:QI:35:GLU:O      | 2.19                     | 0.42              |
| 12:QL:61:THR:C     | 12:QL:63:GLY:H     | 2.27                     | 0.42              |
| 15:QO:71:GLN:HB2   | 15:QO:78:TYR:CE1   | 2.54                     | 0.42              |
| 16:QP:21:VAL:HG21  | 16:QP:59:TRP:NE1   | 2.35                     | 0.42              |
| 19:QS:41:VAL:HG11  | 19:QS:45:VAL:HG13  | 2.02                     | 0.42              |
| 20:QT:14:LYS:O     | 20:QT:15:ARG:C     | 2.62                     | 0.42              |
| 20:QT:99:LEU:O     | 20:QT:100:ILE:CB   | 2.68                     | 0.42              |
| 25:RA:224:G:O6     | 25:RA:419:C:O2'    | 2.36                     | 0.42              |
| 25:RA:302:C:H2'    | 25:RA:303:U:C6     | 2.55                     | 0.42              |
| 25:RA:1638:C:O3'   | 25:RA:2709:G:N2    | 2.53                     | 0.42              |
| 25:RA:1988:C:H2'   | 25:RA:1989:G:O4'   | 2.20                     | 0.42              |
| 28:RE:144:ARG:HB3  | 28:RE:145:LYS:H    | 1.58                     | 0.42              |
| 30:RG:99:MET:O     | 30:RG:103:LEU:HB2  | 2.20                     | 0.42              |
| 31:RH:76:VAL:C     | 31:RH:78:GLY:N     | 2.78                     | 0.42              |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:N    | 2.26                     | 0.42              |
| 32:RI:128:LEU:HA   | 32:RI:128:LEU:HD13 | 1.81                     | 0.42              |
| 33:RN:131:GLN:HE21 | 33:RN:131:GLN:HB3  | 1.57                     | 0.42              |
| 34:RO:31:LYS:HA    | 34:RO:31:LYS:HD3   | 1.92                     | 0.42              |
| 34:RO:71:ARG:HH11  | 39:RT:74:ARG:HH21  | 1.65                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:65:PHE:O     | 36:RQ:66:ILE:CG1   | 2.48                     | 0.42              |
| 38:RS:88:ASP:CG    | 38:RS:89:ARG:H     | 2.28                     | 0.42              |
| 39:RT:89:VAL:O     | 39:RT:90:GLN:CB    | 2.67                     | 0.42              |
| 39:RT:96:ARG:HB2   | 39:RT:96:ARG:CZ    | 2.49                     | 0.42              |
| 40:RU:39:LEU:O     | 40:RU:42:ALA:N     | 2.53                     | 0.42              |
| 40:RU:43:GLY:HA3   | 41:RV:73:SER:OG    | 2.19                     | 0.42              |
| 43:RX:60:ARG:HA    | 43:RX:75:ASP:OD2   | 2.20                     | 0.42              |
| 48:R2:50:ILE:H     | 48:R2:50:ILE:HG13  | 1.64                     | 0.42              |
| 49:R3:37:LEU:N     | 49:R3:37:LEU:HD23  | 2.35                     | 0.42              |
| 50:R4:2:LYS:HD2    | 50:R4:2:LYS:HA     | 1.61                     | 0.42              |
| 55:R9:2:LYS:HD2    | 55:R9:2:LYS:HA     | 1.93                     | 0.42              |
| 1:XA:1112:C:N3     | 3:XC:178:LEU:HD23  | 2.34                     | 0.42              |
| 1:XA:1125:U:OP2    | 1:XA:1145:C:N4     | 2.53                     | 0.42              |
| 1:XA:1302:U:H2'    | 1:XA:1302:U:O2     | 2.19                     | 0.42              |
| 1:XA:1374:A:H2'    | 1:XA:1375:A:O4'    | 2.20                     | 0.42              |
| 1:XA:1453:G:H8     | 20:XT:39:LYS:CE    | 2.33                     | 0.42              |
| 2:XB:97:TRP:HZ3    | 2:XB:172:ILE:HG22  | 1.85                     | 0.42              |
| 2:XB:162:ILE:O     | 2:XB:185:ILE:CG1   | 2.67                     | 0.42              |
| 2:XB:211:ILE:O     | 2:XB:215:LEU:HB2   | 2.20                     | 0.42              |
| 4:XD:94:LEU:HA     | 4:XD:97:LEU:HD12   | 2.01                     | 0.42              |
| 5:XE:79:GLU:OE2    | 8:XH:104:ARG:HA    | 2.20                     | 0.42              |
| 6:XF:36:ARG:NH2    | 6:XF:38:GLU:HG2    | 2.35                     | 0.42              |
| 7:XG:79:ARG:CZ     | 7:XG:82:GLY:HA2    | 2.50                     | 0.42              |
| 8:XH:95:VAL:O      | 8:XH:95:VAL:HG23   | 2.20                     | 0.42              |
| 11:XK:72:ALA:HB1   | 11:XK:77:MET:HG2   | 2.02                     | 0.42              |
| 13:XM:82:MET:HE3   | 13:XM:93:ARG:CG    | 2.50                     | 0.42              |
| 17:XQ:74:LEU:HD13  | 17:XQ:74:LEU:O     | 2.20                     | 0.42              |
| 19:XS:41:VAL:HG11  | 19:XS:45:VAL:HG13  | 2.02                     | 0.42              |
| 20:XT:28:ALA:C     | 20:XT:30:LYS:H     | 2.28                     | 0.42              |
| 25:YA:459:U:OP1    | 53:Y7:39:ARG:HA    | 2.20                     | 0.42              |
| 25:YA:1055:G:H1    | 25:YA:1104:C:H42   | 1.67                     | 0.42              |
| 25:YA:1802:A:H2'   | 25:YA:1803:A:O4'   | 2.20                     | 0.42              |
| 25:YA:2825:C:H6    | 25:YA:2825:C:O5'   | 2.03                     | 0.42              |
| 26:YB:40:U:H1'     | 26:YB:45:A:H61     | 1.85                     | 0.42              |
| 27:YD:12:SER:O     | 27:YD:14:ARG:N     | 2.51                     | 0.42              |
| 27:YD:263:ARG:NH1  | 27:YD:263:ARG:CB   | 2.75                     | 0.42              |
| 28:YE:76:ARG:C     | 28:YE:78:LEU:N     | 2.76                     | 0.42              |
| 29:YF:20:LEU:HD12  | 29:YF:21:ALA:N     | 2.26                     | 0.42              |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:N    | 2.33                     | 0.42              |
| 29:YF:105:VAL:O    | 29:YF:106:ARG:C    | 2.63                     | 0.42              |
| 32:YI:94:ALA:HB2   | 32:YI:116:LEU:HD13 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:30:ILE:HG22  | 33:YN:34:LEU:HD21  | 2.01                     | 0.42              |
| 34:YO:2:ILE:N      | 34:YO:2:ILE:CD1    | 2.82                     | 0.42              |
| 35:YP:65:ARG:HH21  | 54:Y8:15:LYS:HB3   | 1.84                     | 0.42              |
| 35:YP:85:LEU:C     | 35:YP:87:ASP:N     | 2.77                     | 0.42              |
| 37:YR:28:LEU:HD12  | 37:YR:29:LEU:HD12  | 2.02                     | 0.42              |
| 37:YR:34:ILE:HG22  | 37:YR:35:THR:N     | 2.35                     | 0.42              |
| 38:YS:49:VAL:HG21  | 38:YS:77:ALA:HA    | 2.02                     | 0.42              |
| 39:YT:24:PRO:HA    | 39:YT:49:VAL:CG1   | 2.40                     | 0.42              |
| 39:YT:50:ILE:HD11  | 39:YT:102:ILE:HG12 | 2.01                     | 0.42              |
| 39:YT:67:SER:O     | 39:YT:68:TYR:C     | 2.63                     | 0.42              |
| 40:YU:6:THR:HG21   | 40:YU:10:ARG:CZ    | 2.50                     | 0.42              |
| 41:YV:15:GLU:O     | 41:YV:96:ILE:HB    | 2.19                     | 0.42              |
| 41:YV:72:VAL:HG13  | 41:YV:72:VAL:O     | 2.19                     | 0.42              |
| 45:YZ:7:ALA:O      | 45:YZ:62:PRO:HD3   | 2.20                     | 0.42              |
| 51:Y5:35:GLU:O     | 51:Y5:36:CYS:C     | 2.63                     | 0.42              |
| 53:Y7:25:PRO:HA    | 53:Y7:28:ARG:NH2   | 2.35                     | 0.42              |
| 1:QA:410:G:OP2     | 4:QD:25:ARG:HG3    | 2.20                     | 0.42              |
| 1:QA:540:G:H2'     | 1:QA:541:G:O4'     | 2.19                     | 0.42              |
| 2:QB:29:ALA:C      | 2:QB:31:TYR:H      | 2.27                     | 0.42              |
| 2:QB:159:PRO:HB2   | 2:QB:160:ASP:H     | 1.74                     | 0.42              |
| 2:QB:162:ILE:O     | 2:QB:185:ILE:CG1   | 2.67                     | 0.42              |
| 2:QB:163:PHE:CD2   | 2:QB:185:ILE:HD12  | 2.54                     | 0.42              |
| 4:QD:9:CYS:SG      | 4:QD:31:CYS:C      | 2.99                     | 0.42              |
| 4:QD:31:CYS:O      | 4:QD:31:CYS:SG     | 2.78                     | 0.42              |
| 6:QF:36:ARG:CZ     | 6:QF:38:GLU:HG2    | 2.50                     | 0.42              |
| 6:QF:45:LEU:CD1    | 6:QF:59:TYR:HD1    | 2.31                     | 0.42              |
| 6:QF:46:ARG:HG3    | 6:QF:47:ARG:N      | 2.34                     | 0.42              |
| 7:QG:80:VAL:CG1    | 7:QG:81:GLY:N      | 2.83                     | 0.42              |
| 8:QH:21:LYS:O      | 8:QH:22:GLU:C      | 2.63                     | 0.42              |
| 8:QH:53:VAL:HG12   | 8:QH:54:ASP:OD2    | 2.20                     | 0.42              |
| 13:QM:88:ARG:HD2   | 13:QM:88:ARG:O     | 2.19                     | 0.42              |
| 25:RA:30:G:H2'     | 25:RA:31:C:C6      | 2.55                     | 0.42              |
| 25:RA:373:U:H2'    | 25:RA:374:A:C8     | 2.53                     | 0.42              |
| 25:RA:564:C:H2'    | 25:RA:565:C:O4'    | 2.19                     | 0.42              |
| 25:RA:1022:G:C6    | 25:RA:1140:C:C4    | 3.08                     | 0.42              |
| 25:RA:1889:A:H2'   | 25:RA:1890:A:C8    | 2.55                     | 0.42              |
| 25:RA:2103:C:H2'   | 25:RA:2104:G:C8    | 2.55                     | 0.42              |
| 25:RA:2653:U:O2'   | 31:RH:110:SER:HB2  | 2.19                     | 0.42              |
| 28:RE:176:ILE:HD12 | 28:RE:176:ILE:N    | 2.35                     | 0.42              |
| 29:RF:34:TRP:CA    | 35:RP:6:LEU:HD12   | 2.46                     | 0.42              |
| 29:RF:42:ALA:O     | 29:RF:45:ARG:HB2   | 2.18                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:RF:118:ALA:HA   | 29:RF:123:LEU:HB3 | 2.02                     | 0.42              |
| 30:RG:78:SER:O     | 30:RG:80:PHE:N    | 2.53                     | 0.42              |
| 31:RH:128:PRO:CG   | 31:RH:129:THR:H   | 2.33                     | 0.42              |
| 34:RO:16:ALA:HA    | 34:RO:46:ALA:CB   | 2.50                     | 0.42              |
| 35:RP:144:GLU:HA   | 35:RP:145:PRO:HD3 | 1.76                     | 0.42              |
| 38:RS:83:LYS:HE3   | 38:RS:84:GLN:CG   | 2.50                     | 0.42              |
| 38:RS:99:LYS:HE2   | 38:RS:103:GLU:OE2 | 2.20                     | 0.42              |
| 39:RT:123:GLN:O    | 39:RT:124:ASP:C   | 2.63                     | 0.42              |
| 41:RV:21:ARG:HD2   | 41:RV:91:TYR:CE2  | 2.55                     | 0.42              |
| 41:RV:35:LEU:HB2   | 41:RV:37:VAL:CG2  | 2.49                     | 0.42              |
| 45:RZ:28:MET:SD    | 45:RZ:37:VAL:HG11 | 2.60                     | 0.42              |
| 45:RZ:71:VAL:HB    | 45:RZ:88:PHE:CE2  | 2.55                     | 0.42              |
| 47:R1:76:ARG:H     | 47:R1:76:ARG:CD   | 2.29                     | 0.42              |
| 50:R4:68:ARG:HB2   | 50:R4:69:LYS:H    | 1.35                     | 0.42              |
| 53:R7:9:ARG:NH1    | 53:R7:47:ARG:HG3  | 2.35                     | 0.42              |
| 1:XA:372:C:N4      | 1:XA:389:A:H62    | 2.18                     | 0.42              |
| 1:XA:918:A:O2'     | 1:XA:919:A:H5'    | 2.20                     | 0.42              |
| 1:XA:960:U:H4'     | 1:XA:961:U:C5'    | 2.50                     | 0.42              |
| 1:XA:983:A:H5''    | 1:XA:984:C:OP2    | 2.20                     | 0.42              |
| 1:XA:1213:A:N6     | 1:XA:1215:G:N3    | 2.67                     | 0.42              |
| 7:XG:21:VAL:O      | 7:XG:22:LEU:C     | 2.62                     | 0.42              |
| 7:XG:23:VAL:O      | 7:XG:24:THR:C     | 2.62                     | 0.42              |
| 7:XG:24:THR:HA     | 7:XG:27:ILE:HD13  | 2.01                     | 0.42              |
| 9:XI:128:ARG:HD3   | 22:XV:32:C:OP2    | 2.20                     | 0.42              |
| 12:XL:89:ARG:HB3   | 12:XL:97:ARG:HA   | 2.02                     | 0.42              |
| 12:XL:109:GLY:HA3  | 12:XL:121:GLY:O   | 2.20                     | 0.42              |
| 15:XO:54:ARG:NH1   | 15:XO:58:MET:SD   | 2.93                     | 0.42              |
| 17:XQ:76:LEU:HD21  | 17:XQ:79:SER:HB2  | 2.01                     | 0.42              |
| 19:XS:58:VAL:O     | 19:XS:58:VAL:HG23 | 2.20                     | 0.42              |
| 25:YA:143:C:H2'    | 25:YA:144:C:C6    | 2.54                     | 0.42              |
| 25:YA:918:A:C5     | 25:YA:919:G:H1'   | 2.54                     | 0.42              |
| 25:YA:950:G:C6     | 25:YA:951:C:C4    | 3.07                     | 0.42              |
| 25:YA:1871:A:H2'   | 25:YA:1872:A:C8   | 2.55                     | 0.42              |
| 25:YA:2179:C:H2'   | 25:YA:2180:U:C6   | 2.55                     | 0.42              |
| 25:YA:2822:G:O2'   | 25:YA:2825:C:N4   | 2.51                     | 0.42              |
| 25:YA:2854:G:H2'   | 25:YA:2855:C:C6   | 2.55                     | 0.42              |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:H   | 1.83                     | 0.42              |
| 30:YG:27:ASN:HB3   | 30:YG:30:GLU:OE2  | 2.20                     | 0.42              |
| 31:YH:84:SER:OG    | 31:YH:85:LYS:N    | 2.51                     | 0.42              |
| 31:YH:105:LEU:CD1  | 31:YH:105:LEU:N   | 2.81                     | 0.42              |
| 32:YI:133:HIS:HB2  | 32:YI:134:PRO:CD  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:YN:52:VAL:CG1  | 33:YN:53:VAL:N     | 2.82                     | 0.42              |
| 34:YO:17:ARG:HG2  | 34:YO:17:ARG:HH11  | 1.84                     | 0.42              |
| 34:YO:97:ARG:CA   | 34:YO:117:LEU:HD22 | 2.50                     | 0.42              |
| 35:YP:42:SER:O    | 35:YP:43:GLY:C     | 2.63                     | 0.42              |
| 35:YP:49:ARG:HG2  | 35:YP:49:ARG:HH11  | 1.84                     | 0.42              |
| 38:YS:92:TYR:HB2  | 38:YS:98:VAL:HG11  | 2.02                     | 0.42              |
| 39:YT:123:GLN:O   | 39:YT:124:ASP:C    | 2.63                     | 0.42              |
| 40:YU:35:ALA:O    | 40:YU:39:LEU:HG    | 2.19                     | 0.42              |
| 42:YW:74:ALA:O    | 42:YW:75:TYR:CB    | 2.65                     | 0.42              |
| 43:YX:60:ARG:HH22 | 53:Y7:47:ARG:HH12  | 1.68                     | 0.42              |
| 44:YY:20:TYR:CE1  | 44:YY:42:VAL:HA    | 2.55                     | 0.42              |
| 44:YY:51:VAL:CG1  | 44:YY:52:SER:N     | 2.74                     | 0.42              |
| 44:YY:90:LEU:HB2  | 44:YY:91:GLU:H     | 1.53                     | 0.42              |
| 47:Y1:56:GLN:HB2  | 47:Y1:57:GLU:H     | 1.48                     | 0.42              |
| 47:Y1:83:GLU:C    | 47:Y1:83:GLU:CD    | 2.87                     | 0.42              |
| 50:Y4:6:HIS:O     | 50:Y4:7:PRO:C      | 2.63                     | 0.42              |
| 51:Y5:40:LYS:HE2  | 51:Y5:47:PRO:HG2   | 2.02                     | 0.42              |
| 52:Y6:41:PRO:HG3  | 52:Y6:44:ARG:HB2   | 2.01                     | 0.42              |
| 1:QA:1190:G:OP1   | 3:QC:4:LYS:HA      | 2.19                     | 0.41              |
| 1:QA:1213:A:C6    | 1:QA:1215:G:C4     | 3.08                     | 0.41              |
| 1:QA:1359:C:H3'   | 14:QN:35:ARG:HH12  | 1.85                     | 0.41              |
| 2:QB:125:PRO:O    | 2:QB:126:GLU:HB2   | 2.20                     | 0.41              |
| 2:QB:231:GLU:HG3  | 2:QB:233:SER:H     | 1.85                     | 0.41              |
| 4:QD:101:LEU:CD2  | 4:QD:121:VAL:HG11  | 2.50                     | 0.41              |
| 4:QD:111:ALA:HB3  | 4:QD:117:ALA:HB2   | 2.02                     | 0.41              |
| 4:QD:178:VAL:HG12 | 4:QD:179:GLU:N     | 2.35                     | 0.41              |
| 5:QE:56:GLN:C     | 5:QE:58:ALA:H      | 2.27                     | 0.41              |
| 7:QG:140:ASP:O    | 7:QG:142:GLU:N     | 2.52                     | 0.41              |
| 8:QH:29:SER:O     | 8:QH:30:ARG:C      | 2.62                     | 0.41              |
| 10:QJ:29:ARG:O    | 10:QJ:30:SER:HB3   | 2.20                     | 0.41              |
| 13:QM:16:ASP:HB3  | 13:QM:34:LEU:CD1   | 2.49                     | 0.41              |
| 14:QN:22:THR:HB   | 14:QN:33:VAL:CG1   | 2.50                     | 0.41              |
| 15:QO:3:ILE:HD13  | 15:QO:3:ILE:N      | 2.22                     | 0.41              |
| 17:QQ:11:VAL:HG23 | 17:QQ:12:SER:N     | 2.35                     | 0.41              |
| 17:QQ:52:LYS:O    | 17:QQ:53:LEU:C     | 2.63                     | 0.41              |
| 20:QT:96:GLY:O    | 20:QT:97:ALA:CB    | 2.64                     | 0.41              |
| 25:RA:134:C:H2'   | 25:RA:135:G:C8     | 2.55                     | 0.41              |
| 25:RA:1086:A:H3'  | 25:RA:1086:A:N3    | 2.35                     | 0.41              |
| 25:RA:1266:G:O4'  | 42:RW:15:ARG:NH2   | 2.49                     | 0.41              |
| 25:RA:1466:G:H5'  | 25:RA:1467:C:OP1   | 2.20                     | 0.41              |
| 25:RA:1667:G:O2'  | 25:RA:1669:A:N6    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2584:U:H2'  | 25:RA:2585:U:H2'   | 2.01                     | 0.41              |
| 25:RA:2886:G:H2'  | 25:RA:2887:U:H6    | 1.85                     | 0.41              |
| 26:RB:33:G:OP2    | 30:RG:2:PRO:HD3    | 2.20                     | 0.41              |
| 27:RD:35:LYS:HB3  | 27:RD:36:PRO:HA    | 2.00                     | 0.41              |
| 28:RE:7:VAL:CG2   | 28:RE:8:LYS:H      | 2.11                     | 0.41              |
| 30:RG:22:ARG:HH22 | 30:RG:175:LEU:HD21 | 1.85                     | 0.41              |
| 30:RG:73:ALA:O    | 30:RG:84:LYS:O     | 2.38                     | 0.41              |
| 30:RG:126:ASP:CG  | 30:RG:130:ASN:HB2  | 2.45                     | 0.41              |
| 31:RH:146:ALA:HA  | 31:RH:164:TYR:OH   | 2.21                     | 0.41              |
| 32:RI:29:TYR:O    | 32:RI:33:ARG:HB2   | 2.19                     | 0.41              |
| 33:RN:7:LYS:C     | 33:RN:9:VAL:H      | 2.28                     | 0.41              |
| 33:RN:63:THR:HG22 | 33:RN:66:LYS:HZ1   | 1.84                     | 0.41              |
| 34:RO:86:ILE:N    | 34:RO:86:ILE:CD1   | 2.83                     | 0.41              |
| 35:RP:85:LEU:C    | 35:RP:87:ASP:N     | 2.77                     | 0.41              |
| 39:RT:39:ARG:CG   | 39:RT:40:THR:H     | 2.22                     | 0.41              |
| 40:RU:35:ALA:O    | 40:RU:39:LEU:HG    | 2.19                     | 0.41              |
| 40:RU:75:ASN:O    | 40:RU:76:TYR:C     | 2.63                     | 0.41              |
| 43:RX:15:GLU:CD   | 43:RX:15:GLU:H     | 2.27                     | 0.41              |
| 44:RY:97:ARG:NE   | 44:RY:97:ARG:C     | 2.78                     | 0.41              |
| 45:RZ:146:ILE:HA  | 45:RZ:174:VAL:HB   | 2.01                     | 0.41              |
| 47:R1:83:GLU:C    | 47:R1:83:GLU:CD    | 2.87                     | 0.41              |
| 50:R4:38:LYS:HG3  | 50:R4:44:THR:OG1   | 2.20                     | 0.41              |
| 51:R5:40:LYS:HE2  | 51:R5:47:PRO:HG2   | 2.02                     | 0.41              |
| 52:R6:25:LYS:HE2  | 52:R6:27:LYS:CD    | 2.49                     | 0.41              |
| 52:R6:41:PRO:HG3  | 52:R6:44:ARG:HB2   | 2.01                     | 0.41              |
| 53:R7:25:PRO:HA   | 53:R7:28:ARG:NH2   | 2.35                     | 0.41              |
| 54:R8:16:ILE:HD11 | 54:R8:57:ARG:CG    | 2.44                     | 0.41              |
| 1:XA:255:G:OP1    | 17:XQ:69:LYS:NZ    | 2.48                     | 0.41              |
| 1:XA:742:G:OP2    | 15:XO:35:ARG:NH2   | 2.48                     | 0.41              |
| 1:XA:1111:A:N1    | 3:XC:177:THR:HG23  | 2.35                     | 0.41              |
| 3:XC:58:GLU:HB2   | 3:XC:65:ALA:HB3    | 2.01                     | 0.41              |
| 7:XG:18:TYR:CD2   | 7:XG:59:LEU:HD13   | 2.55                     | 0.41              |
| 8:XH:28:ALA:CB    | 8:XH:57:PRO:HB2    | 2.46                     | 0.41              |
| 12:XL:61:THR:C    | 12:XL:63:GLY:H     | 2.27                     | 0.41              |
| 14:XN:3:ARG:CG    | 14:XN:4:LYS:N      | 2.83                     | 0.41              |
| 15:XO:41:GLU:O    | 15:XO:42:HIS:C     | 2.63                     | 0.41              |
| 16:XP:9:PHE:HB3   | 16:XP:10:GLY:H     | 1.64                     | 0.41              |
| 16:XP:45:THR:CG2  | 16:XP:46:PRO:HD2   | 2.47                     | 0.41              |
| 18:XR:37:VAL:O    | 18:XR:38:GLU:C     | 2.63                     | 0.41              |
| 20:XT:74:LYS:C    | 20:XT:76:ALA:N     | 2.76                     | 0.41              |
| 25:YA:83:G:N2     | 25:YA:103:A:OP2    | 2.35                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:464:U:H4'    | 53:Y7:5:TRP:CZ3    | 2.56                     | 0.41              |
| 25:YA:570:G:H2'    | 25:YA:2030:A:C5    | 2.55                     | 0.41              |
| 25:YA:745:G:O2'    | 25:YA:750:A:N6     | 2.53                     | 0.41              |
| 25:YA:1062:G:H8    | 25:YA:1062:G:O5'   | 2.03                     | 0.41              |
| 25:YA:1496:A:C8    | 25:YA:1577:C:O2'   | 2.73                     | 0.41              |
| 25:YA:2291:U:O2'   | 25:YA:2374:C:H1'   | 2.20                     | 0.41              |
| 25:YA:2684:U:O2'   | 34:YO:68:GLU:HG3   | 2.21                     | 0.41              |
| 25:YA:2837:G:H2'   | 25:YA:2838:G:H8    | 1.85                     | 0.41              |
| 27:YD:109:ASP:HB2  | 27:YD:197:GLY:HA2  | 2.03                     | 0.41              |
| 27:YD:165:ILE:O    | 27:YD:166:GLN:NE2  | 2.53                     | 0.41              |
| 27:YD:215:LEU:H    | 27:YD:215:LEU:HG   | 1.59                     | 0.41              |
| 28:YE:4:ILE:HG22   | 28:YE:198:VAL:HB   | 2.02                     | 0.41              |
| 29:YF:53:THR:O     | 29:YF:55:GLY:N     | 2.53                     | 0.41              |
| 29:YF:64:ILE:HG23  | 29:YF:65:TRP:CD1   | 2.54                     | 0.41              |
| 29:YF:80:ALA:O     | 29:YF:83:PHE:HB2   | 2.20                     | 0.41              |
| 30:YG:78:SER:O     | 30:YG:80:PHE:N     | 2.53                     | 0.41              |
| 34:YO:2:ILE:HG12   | 34:YO:8:LEU:HD11   | 2.02                     | 0.41              |
| 34:YO:31:LYS:O     | 34:YO:32:TYR:HD2   | 2.02                     | 0.41              |
| 36:YQ:34:LEU:HD23  | 36:YQ:104:PHE:CD1  | 2.55                     | 0.41              |
| 36:YQ:118:LEU:HD13 | 36:YQ:131:ILE:HG23 | 2.02                     | 0.41              |
| 38:YS:26:LEU:HB3   | 38:YS:87:PHE:HA    | 2.02                     | 0.41              |
| 38:YS:51:ALA:HB3   | 38:YS:73:LEU:HD23  | 2.01                     | 0.41              |
| 39:YT:105:LEU:O    | 39:YT:105:LEU:HG   | 2.19                     | 0.41              |
| 41:YV:44:LYS:C     | 41:YV:46:VAL:N     | 2.77                     | 0.41              |
| 41:YV:47:VAL:HG13  | 41:YV:48:GLY:N     | 2.26                     | 0.41              |
| 1:QA:743:U:H2'     | 1:QA:744:C:C6      | 2.55                     | 0.41              |
| 1:QA:1004:A:P      | 1:QA:1025:U:H3     | 2.43                     | 0.41              |
| 1:QA:1120:G:H2'    | 1:QA:1121:U:C6     | 2.54                     | 0.41              |
| 1:QA:1129:C:H5'    | 1:QA:1130:A:OP1    | 2.20                     | 0.41              |
| 2:QB:5:ILE:HB      | 2:QB:221:LEU:HD23  | 2.01                     | 0.41              |
| 7:QG:17:VAL:HG12   | 7:QG:18:TYR:CD1    | 2.55                     | 0.41              |
| 7:QG:44:TYR:O      | 7:QG:47:CYS:N      | 2.53                     | 0.41              |
| 8:QH:122:ARG:HG3   | 8:QH:122:ARG:HH11  | 1.85                     | 0.41              |
| 13:QM:82:MET:HE3   | 13:QM:93:ARG:CG    | 2.50                     | 0.41              |
| 13:QM:119:GLY:O    | 13:QM:120:LYS:O    | 2.38                     | 0.41              |
| 14:QN:3:ARG:CG     | 14:QN:4:LYS:N      | 2.83                     | 0.41              |
| 14:QN:9:LYS:O      | 14:QN:9:LYS:HG2    | 2.19                     | 0.41              |
| 16:QP:22:THR:HB    | 16:QP:32:TYR:HB3   | 2.03                     | 0.41              |
| 16:QP:45:THR:CG2   | 16:QP:46:PRO:HD2   | 2.47                     | 0.41              |
| 19:QS:10:PHE:CD2   | 19:QS:10:PHE:C     | 2.98                     | 0.41              |
| 20:QT:95:ALA:O     | 20:QT:97:ALA:N     | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:1101:U:H2'  | 25:RA:1102:C:C6   | 2.55                     | 0.41              |
| 25:RA:1474:C:H3'  | 25:RA:1475:G:H8   | 1.86                     | 0.41              |
| 25:RA:1729:A:H2'  | 25:RA:1730:U:H5'' | 2.02                     | 0.41              |
| 25:RA:1777:U:H2'  | 25:RA:1778:U:H6   | 1.85                     | 0.41              |
| 25:RA:2306:C:H2'  | 25:RA:2307:G:H21  | 1.85                     | 0.41              |
| 25:RA:2790:A:C2   | 25:RA:2791:C:H2'  | 2.55                     | 0.41              |
| 28:RE:13:ARG:HH11 | 28:RE:13:ARG:HB2  | 1.81                     | 0.41              |
| 28:RE:35:GLN:HG3  | 28:RE:37:ARG:NH2  | 2.35                     | 0.41              |
| 28:RE:111:ARG:NE  | 28:RE:160:TYR:CE1 | 2.76                     | 0.41              |
| 28:RE:152:LYS:HG2 | 33:RN:78:TYR:CD1  | 2.55                     | 0.41              |
| 29:RF:53:THR:O    | 29:RF:55:GLY:N    | 2.53                     | 0.41              |
| 30:RG:110:ALA:O   | 30:RG:111:LEU:C   | 2.62                     | 0.41              |
| 32:RI:63:ALA:HA   | 32:RI:66:GLU:HG2  | 2.02                     | 0.41              |
| 36:RQ:20:ALA:HA   | 36:RQ:98:LYS:HB3  | 2.02                     | 0.41              |
| 38:RS:30:ARG:NH2  | 38:RS:92:TYR:HD1  | 2.17                     | 0.41              |
| 38:RS:49:VAL:HG21 | 38:RS:77:ALA:HA   | 2.02                     | 0.41              |
| 38:RS:53:SER:HA   | 38:RS:56:LEU:CD2  | 2.50                     | 0.41              |
| 41:RV:44:LYS:C    | 41:RV:46:VAL:H    | 2.28                     | 0.41              |
| 42:RW:19:LEU:HA   | 42:RW:19:LEU:HD12 | 1.79                     | 0.41              |
| 43:RX:57:LEU:HD12 | 43:RX:57:LEU:H    | 1.85                     | 0.41              |
| 43:RX:60:ARG:HH12 | 53:R7:47:ARG:HH22 | 1.67                     | 0.41              |
| 44:RY:41:GLY:O    | 44:RY:42:VAL:C    | 2.63                     | 0.41              |
| 44:RY:91:GLU:CG   | 44:RY:92:ASN:N    | 2.83                     | 0.41              |
| 47:R1:29:GLY:O    | 47:R1:31:GLY:N    | 2.49                     | 0.41              |
| 47:R1:92:LYS:C    | 47:R1:94:LEU:H    | 2.27                     | 0.41              |
| 48:R2:61:LEU:HD23 | 48:R2:64:LEU:HD12 | 2.03                     | 0.41              |
| 1:XA:149:A:H4'    | 1:XA:1450:U:C4    | 2.56                     | 0.41              |
| 1:XA:1135:U:H4'   | 1:XA:1136:U:H5    | 1.84                     | 0.41              |
| 1:XA:1226:C:H2'   | 13:XM:103:THR:HB  | 2.02                     | 0.41              |
| 2:XB:23:ARG:H     | 2:XB:23:ARG:CD    | 2.30                     | 0.41              |
| 2:XB:60:ASP:C     | 2:XB:62:ALA:H     | 2.28                     | 0.41              |
| 2:XB:166:ASP:O    | 2:XB:170:GLU:OE1  | 2.39                     | 0.41              |
| 3:XC:128:PHE:O    | 3:XC:130:VAL:N    | 2.54                     | 0.41              |
| 4:XD:52:SER:O     | 4:XD:55:ALA:N     | 2.52                     | 0.41              |
| 4:XD:96:LEU:O     | 4:XD:97:LEU:C     | 2.63                     | 0.41              |
| 4:XD:115:ARG:O    | 4:XD:116:GLN:C    | 2.63                     | 0.41              |
| 4:XD:198:VAL:CG1  | 4:XD:199:ASN:H    | 2.32                     | 0.41              |
| 5:XE:144:THR:C    | 5:XE:146:ALA:N    | 2.76                     | 0.41              |
| 7:XG:44:TYR:O     | 7:XG:47:CYS:N     | 2.53                     | 0.41              |
| 7:XG:101:LEU:O    | 7:XG:104:LEU:HB2  | 2.20                     | 0.41              |
| 8:XH:105:ARG:O    | 8:XH:107:LEU:N    | 2.47                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:XL:53:ARG:HH12  | 12:XL:92:ASP:HB3  | 1.85                     | 0.41              |
| 14:YN:18:VAL:CG2   | 14:YN:19:ARG:N    | 2.82                     | 0.41              |
| 17:XQ:11:VAL:HG23  | 17:XQ:12:SER:N    | 2.35                     | 0.41              |
| 25:YA:740:U:H2'    | 25:YA:741:G:C8    | 2.55                     | 0.41              |
| 25:YA:862:G:H2'    | 25:YA:863:A:O4'   | 2.20                     | 0.41              |
| 27:YD:9:TYR:CZ     | 27:YD:13:ARG:HD3  | 2.54                     | 0.41              |
| 27:YD:145:VAL:O    | 27:YD:154:LYS:N   | 2.48                     | 0.41              |
| 28:YE:9:VAL:HB     | 28:YE:10:GLY:H    | 1.70                     | 0.41              |
| 28:YE:10:GLY:HA3   | 39:YT:8:LYS:HD3   | 2.02                     | 0.41              |
| 28:YE:167:VAL:CG1  | 28:YE:189:PRO:HD3 | 2.50                     | 0.41              |
| 30:YG:41:GLN:NE2   | 30:YG:154:GLY:O   | 2.52                     | 0.41              |
| 30:YG:180:PHE:C    | 30:YG:182:LYS:N   | 2.76                     | 0.41              |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:N   | 2.26                     | 0.41              |
| 33:YN:58:ASP:HB3   | 33:YN:95:PRO:HB3  | 2.02                     | 0.41              |
| 34:YO:31:LYS:HA    | 34:YO:31:LYS:HD3  | 1.91                     | 0.41              |
| 35:YP:39:LYS:HA    | 35:YP:45:LEU:HD11 | 1.83                     | 0.41              |
| 41:YV:35:LEU:HB2   | 41:YV:37:VAL:CG2  | 2.49                     | 0.41              |
| 42:YW:1:MET:HG3    | 42:YW:2:GLU:N     | 2.36                     | 0.41              |
| 42:YW:8:ARG:HG3    | 42:YW:8:ARG:NH1   | 2.34                     | 0.41              |
| 42:YW:25:ARG:NH1   | 42:YW:25:ARG:CB   | 2.79                     | 0.41              |
| 42:YW:73:ALA:HB3   | 42:YW:106:ILE:CG1 | 2.46                     | 0.41              |
| 45:YZ:100:VAL:HA   | 45:YZ:101:PRO:HD3 | 1.84                     | 0.41              |
| 54:Y8:25:MET:HB3   | 54:Y8:26:LYS:H    | 1.69                     | 0.41              |
| 1:QA:452:A:H2'     | 1:QA:453:A:C8     | 2.55                     | 0.41              |
| 1:QA:538:G:H2'     | 1:QA:539:A:C8     | 2.55                     | 0.41              |
| 1:QA:838:G:C5      | 1:QA:842:C:H1'    | 2.55                     | 0.41              |
| 1:QA:991:U:O4      | 1:QA:1212:U:O2'   | 2.19                     | 0.41              |
| 1:QA:1135:U:H4'    | 1:QA:1136:U:H5    | 1.85                     | 0.41              |
| 1:QA:1316:G:H2'    | 1:QA:1317:C:H5''  | 2.02                     | 0.41              |
| 1:QA:1333:A:H2'    | 1:QA:1334:G:O4'   | 2.21                     | 0.41              |
| 1:QA:1412:C:H2'    | 1:QA:1413:A:C8    | 2.55                     | 0.41              |
| 4:QD:13:ARG:NH2    | 4:QD:36:ARG:CZ    | 2.84                     | 0.41              |
| 4:QD:94:LEU:HA     | 4:QD:97:LEU:HD12  | 2.01                     | 0.41              |
| 5:QE:144:THR:O     | 5:QE:145:LYS:C    | 2.63                     | 0.41              |
| 10:QJ:45:ARG:HB2   | 10:QJ:65:LEU:HB3  | 2.03                     | 0.41              |
| 11:QK:92:GLU:O     | 11:QK:95:ILE:N    | 2.54                     | 0.41              |
| 12:QL:117:ARG:HB3  | 12:QL:122:THR:HB  | 2.02                     | 0.41              |
| 14:QN:41:ARG:HG3   | 14:QN:42:ILE:N    | 2.35                     | 0.41              |
| 15:QO:54:ARG:NH1   | 15:QO:58:MET:SD   | 2.93                     | 0.41              |
| 15:QO:83:GLU:O     | 15:QO:84:LYS:C    | 2.63                     | 0.41              |
| 17:QQ:11:VAL:CG2   | 17:QQ:20:THR:HB   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:QQ:74:LEU:HD13 | 17:QQ:74:LEU:O     | 2.20                     | 0.41              |
| 20:QT:50:GLU:HA   | 20:QT:100:ILE:HG22 | 2.02                     | 0.41              |
| 22:QV:17:C:H2'    | 22:QV:17:C:O2      | 2.20                     | 0.41              |
| 22:QV:23:C:H2'    | 22:QV:24:U:C6      | 2.55                     | 0.41              |
| 25:RA:626:U:H5''  | 25:RA:627:A:H5'    | 2.01                     | 0.41              |
| 25:RA:747:U:N1    | 51:R5:2:ALA:HB3    | 2.35                     | 0.41              |
| 25:RA:900:A:H5'   | 25:RA:901:A:OP2    | 2.19                     | 0.41              |
| 25:RA:997:G:H2'   | 25:RA:998:C:H6     | 1.84                     | 0.41              |
| 25:RA:1227:A:OP1  | 41:RV:84:LYS:NZ    | 2.44                     | 0.41              |
| 25:RA:1676:A:H2'  | 25:RA:1677:A:O4'   | 2.20                     | 0.41              |
| 25:RA:2037:G:C6   | 25:RA:2038:G:C6    | 3.08                     | 0.41              |
| 25:RA:2070:G:H2'  | 25:RA:2071:A:O4'   | 2.20                     | 0.41              |
| 25:RA:2216:G:C4   | 25:RA:2217:G:C8    | 3.09                     | 0.41              |
| 25:RA:2631:G:N3   | 25:RA:2810:A:H2    | 2.18                     | 0.41              |
| 27:RD:13:ARG:HG2  | 27:RD:13:ARG:O     | 2.20                     | 0.41              |
| 27:RD:166:GLN:CA  | 27:RD:166:GLN:NE2  | 2.78                     | 0.41              |
| 31:RH:105:LEU:CD1 | 31:RH:105:LEU:N    | 2.81                     | 0.41              |
| 32:RI:74:ASN:OD1  | 32:RI:74:ASN:N     | 2.52                     | 0.41              |
| 35:RP:18:ARG:HD2  | 35:RP:27:HIS:CD2   | 2.56                     | 0.41              |
| 35:RP:64:LYS:HG3  | 54:R8:25:MET:CE    | 2.50                     | 0.41              |
| 41:RV:16:PRO:HB3  | 41:RV:97:LYS:O     | 2.20                     | 0.41              |
| 44:RY:20:TYR:C    | 44:RY:21:LYS:O     | 2.62                     | 0.41              |
| 51:R5:40:LYS:HE2  | 51:R5:47:PRO:CG    | 2.49                     | 0.41              |
| 1:XA:241:C:C2     | 1:XA:286:G:C2      | 3.08                     | 0.41              |
| 1:XA:1158:C:H4'   | 2:XB:133:LYS:HZ3   | 1.85                     | 0.41              |
| 1:XA:1346:A:O3'   | 1:XA:1347:G:H4'    | 2.20                     | 0.41              |
| 1:XA:1365:G:H2'   | 1:XA:1366:C:H6     | 1.85                     | 0.41              |
| 1:XA:1408:A:O2'   | 25:YA:1916:A:N1    | 2.51                     | 0.41              |
| 2:XB:12:GLU:C     | 2:XB:14:GLY:H      | 2.29                     | 0.41              |
| 2:XB:29:ALA:C     | 2:XB:31:TYR:H      | 2.27                     | 0.41              |
| 3:XC:59:ARG:NH1   | 3:XC:97:LYS:HE3    | 2.34                     | 0.41              |
| 3:XC:76:VAL:CG2   | 3:XC:103:VAL:HG11  | 2.49                     | 0.41              |
| 3:XC:120:VAL:O    | 3:XC:121:ALA:C     | 2.63                     | 0.41              |
| 3:XC:142:MET:HG2  | 3:XC:149:ALA:HB2   | 2.02                     | 0.41              |
| 5:XE:68:GLU:HG3   | 5:XE:70:PRO:HD3    | 2.03                     | 0.41              |
| 5:XE:78:HIS:HE1   | 5:XE:143:ARG:N     | 2.12                     | 0.41              |
| 5:XE:123:LEU:O    | 5:XE:124:GLY:C     | 2.62                     | 0.41              |
| 7:XG:111:ARG:HH11 | 7:XG:111:ARG:CB    | 2.23                     | 0.41              |
| 7:XG:141:VAL:O    | 7:XG:141:VAL:CG1   | 2.65                     | 0.41              |
| 8:XH:38:ILE:CD1   | 8:XH:118:VAL:HG12  | 2.49                     | 0.41              |
| 14:XN:9:LYS:HB3   | 14:XN:9:LYS:HE2    | 1.85                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:XO:50:HIS:O    | 15:XO:53:HIS:HB3   | 2.20                     | 0.41              |
| 17:XQ:22:LEU:HD13 | 17:XQ:41:LYS:HG2   | 2.01                     | 0.41              |
| 18:XR:76:LEU:HD22 | 18:XR:76:LEU:N     | 2.34                     | 0.41              |
| 25:YA:675:A:C8    | 25:YA:804:A:C6     | 3.08                     | 0.41              |
| 25:YA:828:U:H4'   | 25:YA:831:G:N1     | 2.36                     | 0.41              |
| 25:YA:910:A:C5    | 36:YQ:13:GLN:HG3   | 2.56                     | 0.41              |
| 25:YA:1506:C:H5'  | 25:YA:1507:A:OP2   | 2.21                     | 0.41              |
| 25:YA:2086:U:H2'  | 25:YA:2087:G:H8    | 1.85                     | 0.41              |
| 25:YA:2420:C:N4   | 54:Y8:30:ARG:HD2   | 2.35                     | 0.41              |
| 25:YA:2591:C:OP2  | 27:YD:238:GLY:HA3  | 2.21                     | 0.41              |
| 26:YB:28:C:OP2    | 38:YS:33:LYS:HE3   | 2.20                     | 0.41              |
| 26:YB:32:C:C2     | 26:YB:51:G:N2      | 2.88                     | 0.41              |
| 27:YD:14:ARG:CG   | 27:YD:15:PHE:N     | 2.83                     | 0.41              |
| 27:YD:145:VAL:CG1 | 27:YD:146:GLU:N    | 2.84                     | 0.41              |
| 28:YE:35:GLN:HG3  | 28:YE:37:ARG:NH2   | 2.35                     | 0.41              |
| 30:YG:51:ARG:NH1  | 30:YG:51:ARG:CB    | 2.82                     | 0.41              |
| 30:YG:51:ARG:C    | 30:YG:53:LEU:H     | 2.28                     | 0.41              |
| 31:YH:76:VAL:C    | 31:YH:78:GLY:N     | 2.78                     | 0.41              |
| 32:YI:4:ILE:HG22  | 32:YI:16:GLY:HA2   | 2.02                     | 0.41              |
| 32:YI:92:VAL:HG11 | 32:YI:142:VAL:HG11 | 2.01                     | 0.41              |
| 33:YN:21:LYS:O    | 33:YN:22:THR:O     | 2.39                     | 0.41              |
| 33:YN:113:GLY:C   | 33:YN:114:ARG:O    | 2.58                     | 0.41              |
| 35:YP:146:VAL:C   | 35:YP:147:LEU:HD22 | 2.45                     | 0.41              |
| 39:YT:134:GLU:OE1 | 39:YT:135:ALA:N    | 2.53                     | 0.41              |
| 40:YU:97:ASP:HA   | 40:YU:100:VAL:HG23 | 2.01                     | 0.41              |
| 41:YV:16:PRO:HB3  | 41:YV:97:LYS:O     | 2.20                     | 0.41              |
| 41:YV:44:LYS:C    | 41:YV:46:VAL:H     | 2.28                     | 0.41              |
| 43:YX:57:LEU:HD12 | 43:YX:57:LEU:H     | 1.85                     | 0.41              |
| 44:YY:95:LYS:H    | 44:YY:95:LYS:CD    | 2.32                     | 0.41              |
| 47:Y1:80:LEU:O    | 47:Y1:81:LYS:CD    | 2.65                     | 0.41              |
| 50:Y4:38:LYS:HG3  | 50:Y4:44:THR:OG1   | 2.20                     | 0.41              |
| 50:Y4:48:ARG:O    | 50:Y4:49:PHE:C     | 2.63                     | 0.41              |
| 1:QA:410:G:H2'    | 1:QA:429:U:C4      | 2.55                     | 0.41              |
| 1:QA:591:U:H2'    | 1:QA:592:G:H8      | 1.86                     | 0.41              |
| 1:QA:784:C:H4'    | 25:RA:1837:C:OP1   | 2.21                     | 0.41              |
| 1:QA:1095:U:C4    | 1:QA:1096:C:C4     | 3.08                     | 0.41              |
| 3:QC:78:GLY:HA3   | 3:QC:83:ARG:HB2    | 2.03                     | 0.41              |
| 4:QD:96:LEU:O     | 4:QD:97:LEU:C      | 2.64                     | 0.41              |
| 4:QD:115:ARG:O    | 4:QD:116:GLN:C     | 2.63                     | 0.41              |
| 4:QD:198:VAL:CG1  | 4:QD:199:ASN:H     | 2.32                     | 0.41              |
| 7:QG:11:GLN:HG3   | 7:QG:12:LEU:H      | 1.86                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:QG:118:VAL:HG23  | 7:QG:119:ARG:N    | 2.35                     | 0.41              |
| 8:QH:6:ILE:HB      | 8:QH:85:ARG:HH11  | 1.74                     | 0.41              |
| 8:QH:85:ARG:HA     | 8:QH:135:CYS:HB3  | 2.02                     | 0.41              |
| 9:QI:8:GLY:CA      | 9:QI:79:LEU:HD12  | 2.50                     | 0.41              |
| 9:QI:118:LYS:NZ    | 9:QI:118:LYS:HB3  | 2.34                     | 0.41              |
| 10:QJ:40:LEU:HB3   | 10:QJ:41:PRO:HD2  | 2.02                     | 0.41              |
| 11:QK:56:GLY:O     | 11:QK:89:ALA:HB3  | 2.21                     | 0.41              |
| 13:QM:47:ASP:O     | 13:QM:48:LEU:HB3  | 2.20                     | 0.41              |
| 14:QN:48:ALA:HA    | 14:QN:53:LEU:HD12 | 2.02                     | 0.41              |
| 18:QR:67:ALA:O     | 18:QR:68:LYS:C    | 2.62                     | 0.41              |
| 18:QR:84:LYS:H     | 18:QR:84:LYS:HG2  | 1.56                     | 0.41              |
| 19:QS:4:SER:O      | 19:QS:5:LEU:HD13  | 2.20                     | 0.41              |
| 19:QS:41:VAL:HG12  | 19:QS:45:VAL:H    | 1.84                     | 0.41              |
| 20:QT:50:GLU:O     | 20:QT:51:GLU:C    | 2.62                     | 0.41              |
| 24:QX:2:U:HO2'     | 24:QX:3:G:H5'     | 1.82                     | 0.41              |
| 25:RA:190:A:H61    | 25:RA:799:G:HO2'  | 1.67                     | 0.41              |
| 25:RA:297:C:H5''   | 44:RY:85:VAL:CG2  | 2.49                     | 0.41              |
| 25:RA:1468:C:H2'   | 25:RA:1469:A:C8   | 2.55                     | 0.41              |
| 25:RA:1568:G:P     | 27:RD:63:ARG:HH12 | 2.42                     | 0.41              |
| 25:RA:1593:G:H2'   | 25:RA:1594:G:C8   | 2.55                     | 0.41              |
| 25:RA:2250:G:C2    | 36:RQ:82:ARG:HB3  | 2.55                     | 0.41              |
| 25:RA:2513:G:C2    | 25:RA:2514:U:C2   | 3.08                     | 0.41              |
| 25:RA:2529:G:H5''  | 25:RA:2530:A:H5'' | 2.01                     | 0.41              |
| 27:RD:2:ALA:O      | 27:RD:3:VAL:CB    | 2.68                     | 0.41              |
| 27:RD:75:ILE:HG21  | 27:RD:99:ASP:HB2  | 2.02                     | 0.41              |
| 27:RD:269:PHE:CD2  | 27:RD:269:PHE:N   | 2.88                     | 0.41              |
| 28:RE:25:VAL:CG1   | 39:RT:11:GLU:HG2  | 2.50                     | 0.41              |
| 29:RF:108:LYS:O    | 29:RF:109:GLY:C   | 2.61                     | 0.41              |
| 30:RG:53:LEU:CD1   | 30:RG:87:PRO:HB2  | 2.51                     | 0.41              |
| 30:RG:135:LEU:N    | 30:RG:135:LEU:CD1 | 2.84                     | 0.41              |
| 32:RI:129:THR:HG22 | 32:RI:137:PRO:HB3 | 2.02                     | 0.41              |
| 33:RN:21:LYS:O     | 33:RN:22:THR:O    | 2.39                     | 0.41              |
| 33:RN:62:VAL:CG1   | 33:RN:66:LYS:HB2  | 2.51                     | 0.41              |
| 36:RQ:34:LEU:HD23  | 36:RQ:104:PHE:CD1 | 2.55                     | 0.41              |
| 39:RT:134:GLU:O    | 39:RT:135:ALA:CB  | 2.69                     | 0.41              |
| 40:RU:83:LEU:HG    | 40:RU:88:ILE:HG13 | 2.03                     | 0.41              |
| 41:RV:38:LEU:CD2   | 41:RV:39:LEU:N    | 2.82                     | 0.41              |
| 41:RV:38:LEU:CD1   | 41:RV:55:ALA:CB   | 2.99                     | 0.41              |
| 44:RY:5:MET:CE     | 44:RY:32:PRO:HB3  | 2.51                     | 0.41              |
| 45:RZ:117:LEU:HD11 | 45:RZ:172:ALA:HB1 | 2.02                     | 0.41              |
| 50:R4:45:GLY:O     | 50:R4:46:GLN:C    | 2.62                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:429:U:H1'     | 1:XA:430:A:H5''    | 2.01                     | 0.41              |
| 1:XA:445:G:H2'     | 1:XA:446:G:C8      | 2.55                     | 0.41              |
| 1:XA:663:A:H2'     | 1:XA:664:G:O4'     | 2.20                     | 0.41              |
| 1:XA:1374:A:H1'    | 7:XG:31:MET:HE3    | 2.02                     | 0.41              |
| 1:XA:1424:C:H2'    | 1:XA:1425:U:O4'    | 2.21                     | 0.41              |
| 3:XC:88:ARG:NH2    | 3:XC:101:LEU:O     | 2.53                     | 0.41              |
| 4:XD:93:PHE:CE1    | 4:XD:97:LEU:HD11   | 2.55                     | 0.41              |
| 4:XD:101:LEU:C     | 4:XD:101:LEU:HD12  | 2.45                     | 0.41              |
| 7:XG:87:VAL:HG11   | 7:XG:155:ARG:HA    | 2.03                     | 0.41              |
| 9:XI:118:LYS:NZ    | 9:XI:118:LYS:HB3   | 2.34                     | 0.41              |
| 11:XK:20:TYR:N     | 11:XK:31:THR:O     | 2.54                     | 0.41              |
| 12:XL:62:SER:HB2   | 12:XL:64:TYR:CD1   | 2.56                     | 0.41              |
| 13:XM:13:LYS:HA    | 13:XM:44:ARG:CD    | 2.48                     | 0.41              |
| 14:YN:15:LYS:HD3   | 14:YN:15:LYS:HA    | 1.86                     | 0.41              |
| 14:YN:22:THR:HB    | 14:YN:33:VAL:CG1   | 2.50                     | 0.41              |
| 16:XP:21:VAL:HG21  | 16:XP:59:TRP:NE1   | 2.35                     | 0.41              |
| 18:XR:74:ARG:NE    | 18:XR:80:PRO:O     | 2.48                     | 0.41              |
| 25:YA:141(A):C:H2' | 25:YA:142:G:O4'    | 2.21                     | 0.41              |
| 25:YA:250:G:H2'    | 25:YA:251:A:C8     | 2.55                     | 0.41              |
| 25:YA:1161:C:O2'   | 41:YV:8:GLY:HA2    | 2.20                     | 0.41              |
| 25:YA:1533:C:H2'   | 25:YA:1534:G:N7    | 2.35                     | 0.41              |
| 25:YA:2860:A:C8    | 25:YA:2861:G:H1'   | 2.55                     | 0.41              |
| 27:YD:269:PHE:CD2  | 27:YD:269:PHE:N    | 2.88                     | 0.41              |
| 28:YE:186:GLY:C    | 28:YE:188:VAL:H    | 2.28                     | 0.41              |
| 29:YF:34:TRP:CA    | 35:YP:6:LEU:HD12   | 2.47                     | 0.41              |
| 29:YF:160:ASN:CG   | 29:YF:163:VAL:HG23 | 2.45                     | 0.41              |
| 29:YF:176:LEU:HD11 | 29:YF:180:GLY:O    | 2.19                     | 0.41              |
| 30:YG:47:LYS:HE3   | 30:YG:47:LYS:HB2   | 1.80                     | 0.41              |
| 30:YG:146:TYR:C    | 30:YG:148:MET:H    | 2.28                     | 0.41              |
| 31:YH:53:GLU:OE1   | 31:YH:53:GLU:HA    | 2.16                     | 0.41              |
| 33:YN:7:LYS:C      | 33:YN:9:VAL:H      | 2.28                     | 0.41              |
| 33:YN:109:LYS:N    | 33:YN:109:LYS:CD   | 2.83                     | 0.41              |
| 38:YS:83:LYS:HE3   | 38:YS:84:GLN:CG    | 2.49                     | 0.41              |
| 39:YT:77:PRO:C     | 39:YT:79:HIS:H     | 2.29                     | 0.41              |
| 40:YU:75:ASN:O     | 40:YU:76:TYR:C     | 2.63                     | 0.41              |
| 40:YU:83:LEU:HG    | 40:YU:88:ILE:HG13  | 2.02                     | 0.41              |
| 40:YU:98:LEU:C     | 40:YU:100:VAL:N    | 2.77                     | 0.41              |
| 42:YW:68:ARG:O     | 42:YW:110:LYS:N    | 2.46                     | 0.41              |
| 44:YY:6:HIS:O      | 44:YY:7:VAL:CG1    | 2.59                     | 0.41              |
| 45:YZ:72:ARG:NH1   | 45:YZ:97:GLU:O     | 2.51                     | 0.41              |
| 45:YZ:112:ARG:C    | 45:YZ:114:GLY:N    | 2.79                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:QA:79:G:N2        | 1:QA:91:C:O2       | 2.54                     | 0.41              |
| 1:QA:372:C:HO2'     | 1:QA:373:A:P       | 2.43                     | 0.41              |
| 1:QA:895:G:H1       | 1:QA:904:C:N4      | 2.16                     | 0.41              |
| 1:QA:960:U:O2       | 1:QA:960:U:H2'     | 2.18                     | 0.41              |
| 1:QA:1108:G:H5'     | 3:QC:176:HIS:ND1   | 2.34                     | 0.41              |
| 2:QB:97:TRP:HZ3     | 2:QB:172:ILE:HG22  | 1.85                     | 0.41              |
| 2:QB:166:ASP:O      | 2:QB:170:GLU:OE1   | 2.38                     | 0.41              |
| 2:QB:224:GLN:C      | 2:QB:226:ARG:H     | 2.28                     | 0.41              |
| 2:QB:239:VAL:O      | 2:QB:240:GLN:C     | 2.62                     | 0.41              |
| 3:QC:8:ILE:C        | 3:QC:10:PHE:H      | 2.29                     | 0.41              |
| 4:QD:30:LYS:HG3     | 4:QD:35:ARG:CZ     | 2.47                     | 0.41              |
| 6:QF:36:ARG:NH2     | 6:QF:38:GLU:HG2    | 2.35                     | 0.41              |
| 6:QF:92:LYS:NZ      | 6:QF:92:LYS:CB     | 2.84                     | 0.41              |
| 6:QF:101:ALA:HA     | 18:QR:28:GLU:CD    | 2.46                     | 0.41              |
| 7:QG:24:THR:HA      | 7:QG:27:ILE:HD13   | 2.02                     | 0.41              |
| 7:QG:79:ARG:CZ      | 7:QG:82:GLY:HA2    | 2.51                     | 0.41              |
| 7:QG:121:ALA:O      | 7:QG:125:MET:HG3   | 2.21                     | 0.41              |
| 8:QH:11:THR:HA      | 8:QH:14:ARG:NH1    | 2.35                     | 0.41              |
| 10:QJ:45:ARG:HG3    | 10:QJ:45:ARG:HH11  | 1.86                     | 0.41              |
| 12:QL:109:GLY:HA3   | 12:QL:121:GLY:O    | 2.20                     | 0.41              |
| 15:QO:33:THR:O      | 15:QO:34:LEU:C     | 2.63                     | 0.41              |
| 20:QT:32:ALA:O      | 20:QT:33:ILE:C     | 2.61                     | 0.41              |
| 22:QV:13:C:O2'      | 25:RA:1924:C:H4'   | 2.20                     | 0.41              |
| 22:QV:58:A:O2'      | 22:QV:60:U:OP2     | 2.16                     | 0.41              |
| 24:QX:4:C:O2        | 24:QX:4:C:H2'      | 2.20                     | 0.41              |
| 25:RA:747:U:O2'     | 42:RW:88:ARG:HG3   | 2.21                     | 0.41              |
| 25:RA:1045:A:O2'    | 25:RA:1046:A:OP2   | 2.36                     | 0.41              |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:NH2   | 2.33                     | 0.41              |
| 25:RA:1777:U:H2'    | 25:RA:1778:U:C6    | 2.55                     | 0.41              |
| 25:RA:1954:G:O2'    | 25:RA:1956:U:O4    | 2.37                     | 0.41              |
| 25:RA:2030:A:H4'    | 25:RA:2031:A:H8    | 1.84                     | 0.41              |
| 25:RA:2318:G:H1     | 38:RS:2:ALA:N      | 2.19                     | 0.41              |
| 26:RB:43:C:N4       | 26:RB:45:A:C2      | 2.88                     | 0.41              |
| 27:RD:68:LYS:HG3    | 27:RD:68:LYS:O     | 2.20                     | 0.41              |
| 27:RD:158:ALA:O     | 27:RD:196:VAL:HG11 | 2.21                     | 0.41              |
| 28:RE:179:GLU:CB    | 28:RE:181:LEU:HD23 | 2.24                     | 0.41              |
| 29:RF:133:ASN:O     | 29:RF:134:GLY:C    | 2.63                     | 0.41              |
| 31:RH:86:GLU:HG3    | 31:RH:165:ALA:CA   | 2.49                     | 0.41              |
| 32:RI:88:ILE:HG12   | 32:RI:122:GLU:N    | 2.35                     | 0.41              |
| 33:RN:52:VAL:CG1    | 33:RN:53:VAL:N     | 2.82                     | 0.41              |
| 33:RN:94:HIS:C      | 33:RN:95:PRO:O     | 2.64                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RP:146:VAL:C    | 35:RP:147:LEU:HD22 | 2.45                     | 0.41              |
| 37:RR:28:LEU:HD12  | 37:RR:29:LEU:HD12  | 2.01                     | 0.41              |
| 41:RV:38:LEU:CD1   | 41:RV:55:ALA:HB1   | 2.50                     | 0.41              |
| 42:RW:55:ALA:O     | 42:RW:58:ALA:HB3   | 2.21                     | 0.41              |
| 52:R6:6:ARG:HA     | 52:R6:6:ARG:NE     | 2.36                     | 0.41              |
| 1:XA:134:A:H1'     | 1:XA:325:A:C5      | 2.56                     | 0.41              |
| 1:XA:864:A:H2'     | 1:XA:865:A:C8      | 2.55                     | 0.41              |
| 1:XA:908:A:H2'     | 1:XA:909:A:C8      | 2.56                     | 0.41              |
| 1:XA:911:U:H2'     | 1:XA:912:C:C6      | 2.55                     | 0.41              |
| 1:XA:1186:G:H21    | 14:YN:61:TRP:C     | 2.28                     | 0.41              |
| 1:XA:1338:G:C6     | 1:XA:1339:A:C6     | 3.08                     | 0.41              |
| 2:XB:130:ARG:HH22  | 2:XB:138:LEU:HD21  | 1.85                     | 0.41              |
| 2:XB:231:GLU:HG3   | 2:XB:233:SER:H     | 1.86                     | 0.41              |
| 3:XC:59:ARG:HH12   | 3:XC:97:LYS:CE     | 2.33                     | 0.41              |
| 3:XC:70:VAL:HG12   | 3:XC:71:ALA:H      | 1.84                     | 0.41              |
| 4:XD:109:GLY:C     | 4:XD:111:ALA:N     | 2.76                     | 0.41              |
| 4:XD:127:THR:HG23  | 4:XD:130:GLY:O     | 2.19                     | 0.41              |
| 5:XE:26:PHE:CD1    | 5:XE:26:PHE:N      | 2.87                     | 0.41              |
| 6:XF:67:MET:HB2    | 6:XF:68:PRO:CD     | 2.48                     | 0.41              |
| 7:XG:17:VAL:HG12   | 7:XG:18:TYR:CD1    | 2.55                     | 0.41              |
| 7:XG:126:ASP:OD2   | 7:XG:126:ASP:N     | 2.53                     | 0.41              |
| 8:XH:21:LYS:O      | 8:XH:22:GLU:C      | 2.63                     | 0.41              |
| 9:XI:49:PRO:O      | 9:XI:85:LEU:HD21   | 2.20                     | 0.41              |
| 11:XK:56:GLY:O     | 11:XK:89:ALA:HB3   | 2.21                     | 0.41              |
| 14:YN:34:TYR:N     | 14:YN:34:TYR:CD1   | 2.89                     | 0.41              |
| 16:XP:22:THR:HB    | 16:XP:32:TYR:HB3   | 2.02                     | 0.41              |
| 19:XS:39:THR:HG23  | 19:XS:68:GLY:O     | 2.21                     | 0.41              |
| 19:XS:41:VAL:HG13  | 19:XS:44:MET:CB    | 2.38                     | 0.41              |
| 22:XV:17:C:O2      | 22:XV:17:C:H2'     | 2.20                     | 0.41              |
| 25:YA:270(G):C:H2' | 25:YA:270(H):C:C6  | 2.55                     | 0.41              |
| 25:YA:372:G:O2'    | 25:YA:373:U:P      | 2.79                     | 0.41              |
| 25:YA:970:C:H2'    | 25:YA:971:C:C6     | 2.55                     | 0.41              |
| 25:YA:1021:A:C8    | 25:YA:1021:A:C3'   | 3.02                     | 0.41              |
| 25:YA:2002:G:P     | 37:YR:9:LYS:HD3    | 2.61                     | 0.41              |
| 25:YA:2052:G:H2'   | 25:YA:2053:G:C8    | 2.55                     | 0.41              |
| 25:YA:2688:U:O2    | 25:YA:2688:U:H3'   | 2.20                     | 0.41              |
| 25:YA:2707:G:OP1   | 37:YR:68:ARG:NH2   | 2.53                     | 0.41              |
| 27:YD:158:ALA:O    | 27:YD:196:VAL:HG11 | 2.21                     | 0.41              |
| 27:YD:168:ARG:O    | 27:YD:169:GLU:HB2  | 2.19                     | 0.41              |
| 28:YE:63:LEU:CD1   | 28:YE:64:LYS:N     | 2.71                     | 0.41              |
| 28:YE:161:GLY:O    | 28:YE:162:ALA:HB3  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:YH:86:GLU:HG3  | 31:YH:165:ALA:CA  | 2.49                     | 0.41              |
| 32:YI:56:LYS:HE2  | 32:YI:57:ARG:HG2  | 2.03                     | 0.41              |
| 33:YN:9:VAL:HB    | 33:YN:10:GLU:H    | 1.70                     | 0.41              |
| 40:YU:92:ARG:NH2  | 41:YV:11:GLN:O    | 2.53                     | 0.41              |
| 41:YV:21:ARG:HD2  | 41:YV:91:TYR:CE2  | 2.55                     | 0.41              |
| 43:YX:7:VAL:O     | 43:YX:30:VAL:CG1  | 2.67                     | 0.41              |
| 44:YY:5:MET:HE1   | 44:YY:32:PRO:HB3  | 2.02                     | 0.41              |
| 49:Y3:37:LEU:HD23 | 49:Y3:37:LEU:N    | 2.35                     | 0.41              |
| 54:Y8:14:VAL:CG1  | 54:Y8:60:LEU:HD11 | 2.50                     | 0.41              |
| 54:Y8:26:LYS:HD3  | 54:Y8:26:LYS:HA   | 1.86                     | 0.41              |
| 1:QA:501:C:H1'    | 1:QA:549:C:H1'    | 2.03                     | 0.41              |
| 1:QA:767:A:H2'    | 1:QA:768:A:O4'    | 2.21                     | 0.41              |
| 1:QA:836:G:C6     | 1:QA:851:G:C6     | 3.08                     | 0.41              |
| 1:QA:976:G:H5''   | 1:QA:1358:U:O2'   | 2.20                     | 0.41              |
| 1:QA:1128:C:OP1   | 9:QI:66:ARG:NH2   | 2.52                     | 0.41              |
| 2:QB:200:ILE:CG2  | 2:QB:201:ILE:N    | 2.83                     | 0.41              |
| 3:QC:47:LEU:CD1   | 3:QC:76:VAL:HG12  | 2.42                     | 0.41              |
| 4:QD:36:ARG:HA    | 4:QD:37:PRO:HD2   | 1.82                     | 0.41              |
| 7:QG:89:MET:CE    | 7:QG:156:TRP:H    | 2.22                     | 0.41              |
| 7:QG:141:VAL:O    | 7:QG:141:VAL:CG1  | 2.65                     | 0.41              |
| 9:QI:83:ARG:HA    | 9:QI:86:VAL:HG12  | 2.02                     | 0.41              |
| 10:QJ:71:LEU:HD12 | 10:QJ:72:VAL:H    | 1.85                     | 0.41              |
| 11:QK:20:TYR:N    | 11:QK:31:THR:O    | 2.54                     | 0.41              |
| 11:QK:74:ALA:C    | 11:QK:76:GLY:H    | 2.29                     | 0.41              |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:CB   | 2.33                     | 0.41              |
| 12:QL:90:VAL:HG12 | 12:QL:92:ASP:H    | 1.86                     | 0.41              |
| 13:QM:82:MET:HG2  | 13:QM:93:ARG:HG3  | 2.03                     | 0.41              |
| 13:QM:105:THR:O   | 13:QM:106:ASN:C   | 2.64                     | 0.41              |
| 16:QP:8:ARG:HG2   | 16:QP:8:ARG:NH1   | 2.32                     | 0.41              |
| 18:QR:53:ARG:O    | 18:QR:55:ARG:N    | 2.53                     | 0.41              |
| 19:QS:58:VAL:O    | 19:QS:58:VAL:HG23 | 2.20                     | 0.41              |
| 22:QV:21:A:N6     | 22:QV:46:G:H2'    | 2.36                     | 0.41              |
| 25:RA:35:G:H1'    | 25:RA:454:A:C4    | 2.56                     | 0.41              |
| 25:RA:98:G:OP1    | 48:R2:4:SER:HB2   | 2.21                     | 0.41              |
| 25:RA:298:G:N2    | 25:RA:339:U:OP2   | 2.35                     | 0.41              |
| 25:RA:397:G:H1'   | 25:RA:2231:C:O2'  | 2.20                     | 0.41              |
| 25:RA:631:A:H4'   | 35:RP:65:ARG:HA   | 2.03                     | 0.41              |
| 25:RA:956:G:N2    | 25:RA:960:A:OP2   | 2.53                     | 0.41              |
| 25:RA:1430:C:H2'  | 25:RA:1431:U:C6   | 2.56                     | 0.41              |
| 25:RA:1436:G:H1'  | 25:RA:1477:A:O2'  | 2.19                     | 0.41              |
| 25:RA:1812:A:O2'  | 27:RD:45:ASN:HB2  | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1930:G:HO2'  | 25:RA:1931:U:P     | 2.43                     | 0.41              |
| 25:RA:2308:G:N2    | 25:RA:2311:A:H2    | 2.17                     | 0.41              |
| 25:RA:2351:G:O6    | 54:R8:39:LYS:HG2   | 2.21                     | 0.41              |
| 25:RA:2470:G:OP1   | 36:RQ:59:ARG:NH1   | 2.53                     | 0.41              |
| 25:RA:2770:G:H5''  | 25:RA:2771:C:OP2   | 2.20                     | 0.41              |
| 27:RD:134:ARG:HD3  | 27:RD:135:PHE:HE2  | 1.82                     | 0.41              |
| 28:RE:93:VAL:HG21  | 28:RE:180:ASN:HA   | 2.03                     | 0.41              |
| 28:RE:186:GLY:C    | 28:RE:188:VAL:H    | 2.28                     | 0.41              |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:NH1  | 2.30                     | 0.41              |
| 29:RF:160:ASN:CG   | 29:RF:163:VAL:HG23 | 2.45                     | 0.41              |
| 29:RF:183:VAL:HG22 | 29:RF:184:TYR:N    | 2.35                     | 0.41              |
| 30:RG:34:LEU:HD11  | 30:RG:99:MET:CE    | 2.49                     | 0.41              |
| 30:RG:77:ILE:H     | 30:RG:82:LEU:HB2   | 1.84                     | 0.41              |
| 30:RG:117:PHE:CE1  | 30:RG:119:GLY:CA   | 3.03                     | 0.41              |
| 31:RH:45:VAL:O     | 31:RH:45:VAL:CG1   | 2.68                     | 0.41              |
| 31:RH:137:ASP:HB2  | 31:RH:140:LYS:CE   | 2.51                     | 0.41              |
| 34:RO:10:VAL:HG21  | 34:RO:16:ALA:HB3   | 2.03                     | 0.41              |
| 34:RO:48:PRO:O     | 34:RO:50:GLY:N     | 2.53                     | 0.41              |
| 38:RS:64:GLU:O     | 38:RS:68:GLN:HG3   | 2.20                     | 0.41              |
| 39:RT:76:PHE:HA    | 39:RT:77:PRO:HD3   | 1.75                     | 0.41              |
| 40:RU:91:ASP:OD2   | 40:RU:96:ALA:CA    | 2.69                     | 0.41              |
| 41:RV:22:VAL:CG1   | 41:RV:23:GLU:H     | 2.32                     | 0.41              |
| 42:RW:1:MET:HG3    | 42:RW:2:GLU:N      | 2.36                     | 0.41              |
| 44:RY:2:ARG:O      | 44:RY:3:VAL:O      | 2.38                     | 0.41              |
| 44:RY:86:ARG:HD2   | 44:RY:86:ARG:HA    | 1.91                     | 0.41              |
| 47:R1:94:LEU:HA    | 47:R1:94:LEU:HD23  | 1.82                     | 0.41              |
| 50:R4:14:ILE:HA    | 50:R4:31:ILE:O     | 2.21                     | 0.41              |
| 52:R6:8:LYS:O      | 52:R6:9:LEU:HB2    | 2.20                     | 0.41              |
| 54:R8:26:LYS:HA    | 54:R8:26:LYS:HD3   | 1.86                     | 0.41              |
| 1:XA:724:G:C2      | 1:XA:725:G:C8      | 3.08                     | 0.41              |
| 1:XA:1151:A:N3     | 10:XJ:39:PRO:HG3   | 2.36                     | 0.41              |
| 1:XA:1202:G:H1'    | 14:YN:29:ARG:HD2   | 2.02                     | 0.41              |
| 1:XA:1216:G:H5''   | 14:YN:5:ALA:CB     | 2.51                     | 0.41              |
| 2:XB:172:ILE:O     | 2:XB:173:ALA:C     | 2.64                     | 0.41              |
| 5:XE:68:GLU:O      | 5:XE:68:GLU:CG     | 2.68                     | 0.41              |
| 8:XH:26:VAL:O      | 8:XH:27:PRO:C      | 2.63                     | 0.41              |
| 8:XH:122:ARG:HG3   | 8:XH:122:ARG:HH11  | 1.85                     | 0.41              |
| 10:XJ:40:LEU:HB3   | 10:XJ:41:PRO:HD2   | 2.02                     | 0.41              |
| 10:XJ:45:ARG:HG3   | 10:XJ:45:ARG:HH11  | 1.86                     | 0.41              |
| 12:XL:8:ASN:O      | 12:XL:11:VAL:HG23  | 2.20                     | 0.41              |
| 13:XM:77:ASN:O     | 13:XM:78:ILE:C     | 2.62                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:XO:33:THR:O     | 15:XO:34:LEU:C    | 2.63                     | 0.41              |
| 15:XO:83:GLU:O     | 15:XO:84:LYS:C    | 2.63                     | 0.41              |
| 17:XQ:89:LEU:HD23  | 17:XQ:89:LEU:HA   | 1.93                     | 0.41              |
| 19:XS:13:ASP:O     | 19:XS:14:HIS:O    | 2.39                     | 0.41              |
| 19:XS:39:THR:O     | 19:XS:40:ILE:HB   | 2.20                     | 0.41              |
| 25:YA:92:G:H2'     | 25:YA:93:C:H6     | 1.85                     | 0.41              |
| 25:YA:241:A:H4'    | 25:YA:242:G:OP1   | 2.20                     | 0.41              |
| 25:YA:321:G:OP2    | 29:YF:135:LYS:HA  | 2.21                     | 0.41              |
| 25:YA:588:U:O4     | 25:YA:670:A:H1'   | 2.20                     | 0.41              |
| 25:YA:875:G:H2'    | 25:YA:876:C:O4'   | 2.21                     | 0.41              |
| 25:YA:1085:A:O2'   | 25:YA:1086:A:P    | 2.79                     | 0.41              |
| 25:YA:1412:A:H2'   | 25:YA:1413:G:C8   | 2.56                     | 0.41              |
| 25:YA:1605:C:H2'   | 25:YA:1606:G:O4'  | 2.21                     | 0.41              |
| 25:YA:1930:G:N1    | 25:YA:1969:A:OP2  | 2.52                     | 0.41              |
| 25:YA:1991:U:H2'   | 25:YA:1992:G:H5'' | 2.01                     | 0.41              |
| 25:YA:2154:G:H2'   | 25:YA:2155:G:C8   | 2.55                     | 0.41              |
| 25:YA:2292:C:P     | 38:YS:17:ARG:HH22 | 2.44                     | 0.41              |
| 27:YD:117:VAL:HG22 | 27:YD:118:VAL:N   | 2.35                     | 0.41              |
| 27:YD:182:LEU:N    | 27:YD:272:ALA:HB3 | 2.32                     | 0.41              |
| 29:YF:129:PHE:O    | 29:YF:142:TRP:HD1 | 2.03                     | 0.41              |
| 29:YF:133:ASN:O    | 29:YF:134:GLY:C   | 2.63                     | 0.41              |
| 31:YH:146:ALA:HB2  | 31:YH:164:TYR:OH  | 2.21                     | 0.41              |
| 33:YN:94:HIS:C     | 33:YN:95:PRO:O    | 2.64                     | 0.41              |
| 34:YO:48:PRO:O     | 34:YO:50:GLY:N    | 2.54                     | 0.41              |
| 34:YO:71:ARG:HH11  | 39:YT:74:ARG:HH21 | 1.65                     | 0.41              |
| 34:YO:112:MET:HE2  | 34:YO:112:MET:N   | 2.34                     | 0.41              |
| 37:YR:55:ALA:HA    | 37:YR:80:PHE:CE2  | 2.55                     | 0.41              |
| 38:YS:66:ALA:HA    | 38:YS:69:VAL:CG1  | 2.51                     | 0.41              |
| 39:YT:76:PHE:HA    | 39:YT:77:PRO:HD3  | 1.75                     | 0.41              |
| 40:YU:39:LEU:O     | 40:YU:42:ALA:N    | 2.53                     | 0.41              |
| 41:YV:29:PRO:C     | 41:YV:61:VAL:HG22 | 2.45                     | 0.41              |
| 44:YY:41:GLY:O     | 44:YY:42:VAL:C    | 2.63                     | 0.41              |
| 44:YY:87:LYS:HB2   | 44:YY:87:LYS:HZ2  | 1.85                     | 0.41              |
| 49:Y3:37:LEU:HD12  | 49:Y3:43:ILE:CG2  | 2.50                     | 0.41              |
| 1:QA:190:G:H4'     | 1:QA:191(A):G:OP2 | 2.20                     | 0.41              |
| 1:QA:484:G:H4'     | 1:QA:485:G:O5'    | 2.21                     | 0.41              |
| 1:QA:520:A:O2'     | 12:QL:73:GLU:HG2  | 2.21                     | 0.41              |
| 1:QA:538:G:H5''    | 12:QL:114:LYS:HB2 | 2.02                     | 0.41              |
| 1:QA:539:A:OP2     | 12:QL:115:LYS:HE3 | 2.20                     | 0.41              |
| 1:QA:757:U:H2'     | 1:QA:758:G:O4'    | 2.21                     | 0.41              |
| 1:QA:828:A:H2'     | 1:QA:829:G:O4'    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:973:G:C4     | 10:QJ:55:LYS:HE2   | 2.55                     | 0.41              |
| 1:QA:976:G:N2     | 1:QA:1362(A):C:OP2 | 2.37                     | 0.41              |
| 1:QA:992:U:H1'    | 1:QA:993:G:OP2     | 2.21                     | 0.41              |
| 1:QA:1118:C:OP1   | 9:QI:104:ARG:NH1   | 2.54                     | 0.41              |
| 1:QA:1227:A:OP2   | 13:QM:111:LYS:HE3  | 2.21                     | 0.41              |
| 1:QA:1330:U:H4'   | 13:QM:23:TYR:CZ    | 2.55                     | 0.41              |
| 2:QB:97:TRP:O     | 2:QB:98:LEU:C      | 2.64                     | 0.41              |
| 2:QB:115:LEU:O    | 2:QB:119:GLU:N     | 2.54                     | 0.41              |
| 2:QB:168:THR:CG2  | 2:QB:192:SER:HB2   | 2.51                     | 0.41              |
| 3:QC:55:VAL:HG12  | 3:QC:55:VAL:O      | 2.20                     | 0.41              |
| 3:QC:120:VAL:O    | 3:QC:121:ALA:C     | 2.63                     | 0.41              |
| 4:QD:30:LYS:HB3   | 4:QD:35:ARG:CG     | 2.36                     | 0.41              |
| 5:QE:128:PRO:O    | 5:QE:129:ILE:C     | 2.63                     | 0.41              |
| 6:QF:3:ARG:HB3    | 6:QF:93:SER:CB     | 2.47                     | 0.41              |
| 7:QG:22:LEU:O     | 7:QG:25:ALA:HB3    | 2.21                     | 0.41              |
| 7:QG:78:ARG:NH1   | 7:QG:78:ARG:CG     | 2.84                     | 0.41              |
| 7:QG:92:SER:HB3   | 7:QG:95:ARG:HB2    | 2.03                     | 0.41              |
| 9:QI:91:ASP:C     | 9:QI:93:ARG:H      | 2.29                     | 0.41              |
| 9:QI:128:ARG:HH21 | 22:QV:35:A:P       | 2.44                     | 0.41              |
| 11:QK:22:HIS:HB3  | 11:QK:29:ILE:HG22  | 2.03                     | 0.41              |
| 14:QN:18:VAL:CG2  | 14:QN:19:ARG:H     | 2.32                     | 0.41              |
| 17:QQ:89:LEU:HD23 | 17:QQ:89:LEU:HA    | 1.93                     | 0.41              |
| 25:RA:196:A:O5'   | 35:RP:46:LYS:NZ    | 2.48                     | 0.41              |
| 25:RA:372:G:O2'   | 25:RA:373:U:P      | 2.78                     | 0.41              |
| 25:RA:512:G:HO2'  | 25:RA:513:A:P      | 2.43                     | 0.41              |
| 25:RA:2025:C:H2'  | 25:RA:2026:C:C6    | 2.56                     | 0.41              |
| 25:RA:2376:A:H2'  | 25:RA:2377:A:O4'   | 2.21                     | 0.41              |
| 25:RA:2391:G:OP2  | 54:R8:32:LEU:HD13  | 2.21                     | 0.41              |
| 28:RE:71:GLY:O    | 28:RE:72:VAL:C     | 2.63                     | 0.41              |
| 28:RE:134:ILE:C   | 28:RE:134:ILE:CD1  | 2.94                     | 0.41              |
| 28:RE:167:VAL:CG1 | 28:RE:189:PRO:HD3  | 2.50                     | 0.41              |
| 29:RF:46:ARG:CG   | 29:RF:46:ARG:NH1   | 2.72                     | 0.41              |
| 30:RG:47:LYS:HB2  | 30:RG:47:LYS:HE3   | 1.80                     | 0.41              |
| 35:RP:55:ARG:HG2  | 35:RP:55:ARG:NH2   | 2.36                     | 0.41              |
| 37:RR:47:PHE:O    | 37:RR:51:LEU:HD23  | 2.21                     | 0.41              |
| 39:RT:28:VAL:HG23 | 39:RT:87:ASP:O     | 2.21                     | 0.41              |
| 40:RU:6:THR:HG21  | 40:RU:10:ARG:CZ    | 2.50                     | 0.41              |
| 40:RU:33:ARG:O    | 40:RU:37:GLU:HB2   | 2.21                     | 0.41              |
| 40:RU:76:TYR:O    | 40:RU:80:ILE:HG12  | 2.21                     | 0.41              |
| 40:RU:89:GLU:C    | 40:RU:90:VAL:O     | 2.62                     | 0.41              |
| 44:RY:13:VAL:O    | 44:RY:24:VAL:HA    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:R2:27:GLU:N    | 48:R2:27:GLU:CD    | 2.77                     | 0.41              |
| 48:R2:41:ILE:HD12 | 48:R2:43:GLN:N     | 2.35                     | 0.41              |
| 50:R4:12:ALA:HB1  | 50:R4:30:GLU:N     | 2.35                     | 0.41              |
| 1:XA:201:C:N4     | 1:XA:209:U:O2      | 2.54                     | 0.41              |
| 1:XA:427:U:O2'    | 1:XA:541:G:OP1     | 2.38                     | 0.41              |
| 1:XA:756:C:H2'    | 1:XA:757:U:O4'     | 2.21                     | 0.41              |
| 1:XA:1222:G:OP1   | 19:XS:77:THR:HG21  | 2.21                     | 0.41              |
| 1:XA:1285:A:H4'   | 1:XA:1286:A:C5'    | 2.51                     | 0.41              |
| 1:XA:1399:C:C2    | 1:XA:1401:G:C5     | 3.09                     | 0.41              |
| 1:XA:1517:G:H1'   | 25:YA:1919:A:O3'   | 2.20                     | 0.41              |
| 2:XB:62:ALA:O     | 2:XB:65:GLY:N      | 2.53                     | 0.41              |
| 2:XB:200:ILE:CG2  | 2:XB:201:ILE:N     | 2.83                     | 0.41              |
| 3:XC:19:GLU:HA    | 3:XC:54:ARG:NH1    | 2.14                     | 0.41              |
| 4:XD:101:LEU:CD2  | 4:XD:121:VAL:HG11  | 2.50                     | 0.41              |
| 5:XE:51:VAL:CB    | 5:XE:52:PRO:HD3    | 2.38                     | 0.41              |
| 8:XH:133:LEU:C    | 8:XH:133:LEU:HD23  | 2.46                     | 0.41              |
| 11:XK:21:ILE:HD13 | 11:XK:84:VAL:HG12  | 2.02                     | 0.41              |
| 11:XK:62:GLN:C    | 11:XK:64:ALA:N     | 2.76                     | 0.41              |
| 11:XK:74:ALA:C    | 11:XK:76:GLY:H     | 2.29                     | 0.41              |
| 11:XK:124:LYS:HB3 | 11:XK:125:PHE:CD1  | 2.47                     | 0.41              |
| 12:XL:25:PRO:HD2  | 12:XL:97:ARG:HH11  | 1.86                     | 0.41              |
| 12:XL:38:THR:HG22 | 12:XL:57:LYS:HB3   | 2.01                     | 0.41              |
| 13:XM:15:VAL:O    | 13:XM:19:LEU:HD22  | 2.21                     | 0.41              |
| 16:XP:20:VAL:CG2  | 16:XP:32:TYR:CD2   | 3.04                     | 0.41              |
| 16:XP:59:TRP:O    | 16:XP:60:LEU:C     | 2.63                     | 0.41              |
| 17:XQ:11:VAL:HG23 | 17:XQ:12:SER:H     | 1.85                     | 0.41              |
| 17:XQ:52:LYS:O    | 17:XQ:53:LEU:C     | 2.62                     | 0.41              |
| 17:XQ:77:VAL:O    | 17:XQ:77:VAL:HG12  | 2.20                     | 0.41              |
| 18:XR:40:LEU:C    | 18:XR:42:ARG:N     | 2.76                     | 0.41              |
| 18:XR:53:ARG:O    | 18:XR:55:ARG:N     | 2.53                     | 0.41              |
| 18:XR:74:ARG:HG2  | 18:XR:79:LEU:HB2   | 2.01                     | 0.41              |
| 19:XS:7:LYS:CG    | 19:XS:8:GLY:N      | 2.83                     | 0.41              |
| 20:XT:10:LEU:O    | 20:XT:12:ALA:N     | 2.54                     | 0.41              |
| 25:YA:1368:G:C2   | 25:YA:1369:G:C8    | 3.09                     | 0.41              |
| 25:YA:1654:A:P    | 37:YR:2:ARG:HD2    | 2.60                     | 0.41              |
| 25:YA:1704:G:H2'  | 25:YA:1705:G:H8    | 1.85                     | 0.41              |
| 25:YA:1798:U:H5'' | 27:YD:259:THR:HG22 | 2.03                     | 0.41              |
| 25:YA:2353:G:H1'  | 46:Y0:34:GLY:HA3   | 2.02                     | 0.41              |
| 25:YA:2712:U:H1'  | 25:YA:2712(A):A:N7 | 2.36                     | 0.41              |
| 27:YD:197:GLY:O   | 27:YD:198:ASN:HB3  | 2.21                     | 0.41              |
| 30:YG:95:ARG:CA   | 30:YG:99:MET:HB3   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:YP:96:THR:O    | 35:YP:97:PRO:C    | 2.63                     | 0.41              |
| 38:YS:53:SER:HA   | 38:YS:56:LEU:CD2  | 2.50                     | 0.41              |
| 39:YT:28:VAL:HG23 | 39:YT:87:ASP:O    | 2.21                     | 0.41              |
| 40:YU:92:ARG:HD2  | 41:YV:11:GLN:CD   | 2.43                     | 0.41              |
| 41:YV:38:LEU:O    | 41:YV:51:VAL:HA   | 2.21                     | 0.41              |
| 42:YW:14:PRO:HG3  | 42:YW:101:SER:OG  | 2.21                     | 0.41              |
| 42:YW:55:ALA:O    | 42:YW:58:ALA:HB3  | 2.20                     | 0.41              |
| 43:YX:83:VAL:CG1  | 43:YX:87:GLN:HB2  | 2.50                     | 0.41              |
| 44:YY:97:ARG:NE   | 44:YY:97:ARG:C    | 2.78                     | 0.41              |
| 47:Y1:63:ALA:C    | 47:Y1:65:SER:N    | 2.78                     | 0.41              |
| 47:Y1:86:SER:O    | 47:Y1:89:GLU:HB2  | 2.21                     | 0.41              |
| 51:Y5:41:PRO:HA   | 51:Y5:42:PRO:HD3  | 1.82                     | 0.41              |
| 1:QA:584:G:H2'    | 1:QA:585:G:H8     | 1.82                     | 0.41              |
| 1:QA:1230:C:H2'   | 1:QA:1231:G:H8    | 1.85                     | 0.41              |
| 3:QC:108:ASN:HB3  | 3:QC:111:LEU:CG   | 2.51                     | 0.41              |
| 4:QD:88:VAL:O     | 4:QD:89:THR:C     | 2.63                     | 0.41              |
| 4:QD:199:ASN:C    | 4:QD:201:GLN:N    | 2.79                     | 0.41              |
| 7:QG:101:LEU:O    | 7:QG:104:LEU:HB2  | 2.20                     | 0.41              |
| 12:QL:89:ARG:HB3  | 12:QL:97:ARG:HA   | 2.02                     | 0.41              |
| 13:QM:20:THR:C    | 13:QM:22:ILE:H    | 2.29                     | 0.41              |
| 13:QM:80:ARG:NH1  | 19:QS:65:ASN:O    | 2.51                     | 0.41              |
| 13:QM:110:ARG:HG3 | 13:QM:110:ARG:O   | 2.20                     | 0.41              |
| 14:QN:15:LYS:O    | 14:QN:16:PHE:C    | 2.63                     | 0.41              |
| 15:QO:25:THR:CG2  | 15:QO:70:LEU:HB2  | 2.48                     | 0.41              |
| 16:QP:6:LEU:N     | 16:QP:6:LEU:CD1   | 2.84                     | 0.41              |
| 25:RA:945:A:C4    | 25:RA:2448:A:C2   | 3.08                     | 0.41              |
| 25:RA:1140:C:P    | 33:RN:66:LYS:HZ3  | 2.44                     | 0.41              |
| 25:RA:2867:G:O2'  | 25:RA:2868:A:O5'  | 2.39                     | 0.41              |
| 27:RD:197:GLY:O   | 27:RD:198:ASN:HB3 | 2.21                     | 0.41              |
| 28:RE:179:GLU:C   | 28:RE:181:LEU:H   | 2.28                     | 0.41              |
| 29:RF:28:ILE:HD12 | 29:RF:28:ILE:C    | 2.46                     | 0.41              |
| 30:RG:51:ARG:C    | 30:RG:53:LEU:H    | 2.29                     | 0.41              |
| 30:RG:61:ALA:CB   | 30:RG:67:LYS:HA   | 2.50                     | 0.41              |
| 30:RG:146:TYR:C   | 30:RG:148:MET:H   | 2.28                     | 0.41              |
| 33:RN:133:GLN:CB  | 33:RN:135:PRO:HD3 | 2.42                     | 0.41              |
| 34:RO:2:ILE:HG12  | 34:RO:8:LEU:HD11  | 2.02                     | 0.41              |
| 35:RP:42:SER:O    | 35:RP:43:GLY:C    | 2.63                     | 0.41              |
| 36:RQ:20:ALA:HB1  | 36:RQ:99:PRO:CG   | 2.51                     | 0.41              |
| 36:RQ:80:GLU:C    | 36:RQ:81:VAL:CG1  | 2.89                     | 0.41              |
| 36:RQ:139:GLU:CG  | 36:RQ:140:ALA:N   | 2.84                     | 0.41              |
| 42:RW:50:VAL:O    | 42:RW:53:SER:N    | 2.50                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RX:53:LYS:HZ1   | 43:RX:55:ASN:CG    | 2.29                     | 0.41              |
| 43:RX:83:VAL:CG1   | 43:RX:87:GLN:HB2   | 2.50                     | 0.41              |
| 44:RY:97:ARG:HH21  | 44:RY:98:VAL:CG2   | 2.33                     | 0.41              |
| 45:RZ:14:LYS:HA    | 45:RZ:15:PRO:HD3   | 1.92                     | 0.41              |
| 47:R1:18:ILE:O     | 47:R1:18:ILE:HG22  | 2.21                     | 0.41              |
| 54:R8:14:VAL:CG1   | 54:R8:60:LEU:HD11  | 2.51                     | 0.41              |
| 1:XA:962:C:H1'     | 1:XA:1201:A:N6     | 2.36                     | 0.41              |
| 1:XA:1483:A:H1'    | 25:YA:1948:G:H1'   | 2.03                     | 0.41              |
| 2:XB:115:LEU:O     | 2:XB:119:GLU:N     | 2.54                     | 0.41              |
| 2:XB:224:GLN:C     | 2:XB:226:ARG:H     | 2.28                     | 0.41              |
| 4:XD:111:ALA:HB3   | 4:XD:117:ALA:HB2   | 2.02                     | 0.41              |
| 4:XD:209:ARG:NE    | 4:XD:209:ARG:HA    | 2.36                     | 0.41              |
| 7:XG:80:VAL:CG1    | 7:XG:81:GLY:N      | 2.83                     | 0.41              |
| 10:XJ:29:ARG:O     | 10:XJ:30:SER:HB3   | 2.20                     | 0.41              |
| 13:XM:117:VAL:O    | 13:XM:119:GLY:N    | 2.53                     | 0.41              |
| 13:XM:119:GLY:O    | 13:XM:120:LYS:C    | 2.63                     | 0.41              |
| 16:XP:1:MET:O      | 16:XP:2:VAL:C      | 2.63                     | 0.41              |
| 19:XS:10:PHE:CD2   | 19:XS:10:PHE:C     | 2.98                     | 0.41              |
| 20:XT:89:ARG:HH12  | 20:XT:106:ALA:CB   | 2.34                     | 0.41              |
| 24:XX:2:U:HO2'     | 24:XX:3:G:H5'      | 1.81                     | 0.41              |
| 25:YA:143:C:H2'    | 25:YA:144:C:H6     | 1.85                     | 0.41              |
| 25:YA:223:A:N1     | 25:YA:407:G:O2'    | 2.48                     | 0.41              |
| 25:YA:787:U:H5''   | 25:YA:788:A:H5'    | 2.02                     | 0.41              |
| 25:YA:829:A:N7     | 25:YA:2248:C:H5'   | 2.36                     | 0.41              |
| 25:YA:856:C:H1'    | 46:Y0:27:GLU:HB3   | 2.03                     | 0.41              |
| 25:YA:1101:U:H2'   | 25:YA:1102:C:H6    | 1.85                     | 0.41              |
| 25:YA:1111:A:O2'   | 25:YA:1112:G:H4'   | 2.20                     | 0.41              |
| 25:YA:2056:G:H2'   | 25:YA:2056:G:N3    | 2.36                     | 0.41              |
| 25:YA:2711:A:C5'   | 25:YA:2712:U:H5'   | 2.49                     | 0.41              |
| 27:YD:134:ARG:H    | 27:YD:134:ARG:HG3  | 1.55                     | 0.41              |
| 28:YE:24:THR:HB    | 28:YE:184:VAL:HG23 | 2.02                     | 0.41              |
| 30:YG:22:ARG:HH22  | 30:YG:175:LEU:HD21 | 1.85                     | 0.41              |
| 31:YH:59:ARG:CG    | 31:YH:59:ARG:NH1   | 2.79                     | 0.41              |
| 33:YN:62:VAL:CG1   | 33:YN:66:LYS:HB2   | 2.50                     | 0.41              |
| 35:YP:101:VAL:HG23 | 35:YP:106:LEU:HB3  | 2.03                     | 0.41              |
| 44:YY:2:ARG:O      | 44:YY:3:VAL:O      | 2.38                     | 0.41              |
| 44:YY:95:LYS:HB2   | 44:YY:95:LYS:HZ1   | 1.86                     | 0.41              |
| 45:YZ:5:LEU:O      | 45:YZ:5:LEU:HD13   | 2.21                     | 0.41              |
| 52:Y6:27:LYS:NZ    | 52:Y6:27:LYS:CB    | 2.73                     | 0.41              |
| 1:QA:192:U:H2'     | 1:QA:193:C:C6      | 2.56                     | 0.41              |
| 1:QA:222:U:H2'     | 1:QA:223:U:H6      | 1.81                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:277:C:HO2'    | 1:QA:282:A:HO2'   | 1.67                     | 0.41              |
| 1:QA:557:G:C6      | 1:QA:558:G:C6     | 3.09                     | 0.41              |
| 1:QA:560:U:H6      | 1:QA:560:U:H2'    | 1.74                     | 0.41              |
| 1:QA:614:A:OP1     | 4:QD:85:LYS:NZ    | 2.54                     | 0.41              |
| 1:QA:792:A:N3      | 1:QA:792:A:H2'    | 2.36                     | 0.41              |
| 1:QA:1125:U:O4     | 10:QJ:5:ARG:HD3   | 2.21                     | 0.41              |
| 2:QB:32:ILE:HD13   | 2:QB:190:THR:HG21 | 2.03                     | 0.41              |
| 2:QB:60:ASP:C      | 2:QB:62:ALA:H     | 2.28                     | 0.41              |
| 2:QB:62:ALA:O      | 2:QB:65:GLY:N     | 2.53                     | 0.41              |
| 2:QB:223:ILE:O     | 2:QB:226:ARG:HB3  | 2.21                     | 0.41              |
| 4:QD:15:GLU:N      | 4:QD:15:GLU:OE1   | 2.54                     | 0.41              |
| 4:QD:107:ARG:C     | 4:QD:109:GLY:N    | 2.79                     | 0.41              |
| 4:QD:199:ASN:OD1   | 4:QD:201:GLN:HB3  | 2.21                     | 0.41              |
| 5:QE:10:MET:CE     | 5:QE:13:ILE:HD13  | 2.51                     | 0.41              |
| 5:QE:32:VAL:CG2    | 5:QE:58:ALA:HB1   | 2.51                     | 0.41              |
| 5:QE:68:GLU:O      | 5:QE:68:GLU:CG    | 2.68                     | 0.41              |
| 7:QG:21:VAL:O      | 7:QG:22:LEU:C     | 2.62                     | 0.41              |
| 8:QH:38:ILE:CD1    | 8:QH:118:VAL:HG12 | 2.49                     | 0.41              |
| 9:QI:88:TYR:O      | 9:QI:89:ASN:HB2   | 2.20                     | 0.41              |
| 12:QL:8:ASN:O      | 12:QL:11:VAL:HG23 | 2.20                     | 0.41              |
| 12:QL:21:LYS:N     | 12:QL:21:LYS:CD   | 2.83                     | 0.41              |
| 12:QL:53:ARG:HH12  | 12:QL:92:ASP:HB3  | 1.85                     | 0.41              |
| 12:QL:62:SER:HB2   | 12:QL:64:TYR:CD1  | 2.56                     | 0.41              |
| 13:QM:15:VAL:O     | 13:QM:19:LEU:HD22 | 2.21                     | 0.41              |
| 13:QM:117:VAL:O    | 13:QM:119:GLY:N   | 2.53                     | 0.41              |
| 14:QN:6:LEU:HD23   | 14:QN:6:LEU:C     | 2.45                     | 0.41              |
| 15:QO:13:GLN:C     | 15:QO:15:PHE:N    | 2.79                     | 0.41              |
| 15:QO:69:TYR:CZ    | 15:QO:73:GLU:HG3  | 2.56                     | 0.41              |
| 17:QQ:13:ASP:C     | 17:QQ:15:MET:N    | 2.77                     | 0.41              |
| 17:QQ:85:VAL:HG12  | 17:QQ:85:VAL:O    | 2.20                     | 0.41              |
| 18:QR:52:PRO:HG2   | 18:QR:55:ARG:HG2  | 2.03                     | 0.41              |
| 19:QS:29:ARG:HG2   | 19:QS:29:ARG:NH1  | 2.36                     | 0.41              |
| 19:QS:39:THR:HG23  | 19:QS:68:GLY:O    | 2.21                     | 0.41              |
| 25:RA:270(I):G:H2' | 25:RA:270(J):G:C8 | 2.56                     | 0.41              |
| 25:RA:271(B):G:H2' | 25:RA:421:U:OP2   | 2.21                     | 0.41              |
| 25:RA:328:U:H4'    | 44:RY:68:HIS:CD2  | 2.56                     | 0.41              |
| 25:RA:458:G:O2'    | 53:R7:39:ARG:HD3  | 2.20                     | 0.41              |
| 25:RA:515:A:H1'    | 25:RA:581:C:H1'   | 2.03                     | 0.41              |
| 25:RA:774:A:H2     | 25:RA:787:U:O2'   | 2.04                     | 0.41              |
| 25:RA:846:C:C2     | 25:RA:847:U:H5    | 2.39                     | 0.41              |
| 25:RA:1071:G:H22   | 25:RA:1091:G:H8   | 1.68                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1248:G:C4   | 40:RU:3:ARG:HG3    | 2.56                     | 0.41              |
| 25:RA:1454:U:H5'  | 37:RR:63:ARG:NE    | 2.24                     | 0.41              |
| 25:RA:1756:G:H4'  | 25:RA:1758:G:O4'   | 2.21                     | 0.41              |
| 25:RA:1799:G:H5'  | 25:RA:1819:A:H61   | 1.85                     | 0.41              |
| 25:RA:2206:C:H2'  | 25:RA:2207:C:C6    | 2.56                     | 0.41              |
| 25:RA:2286:A:H3'  | 52:R6:31:PRO:CG    | 2.51                     | 0.41              |
| 25:RA:2734:A:H3'  | 25:RA:2735:G:H8    | 1.86                     | 0.41              |
| 25:RA:2822:G:O2'  | 25:RA:2824:C:OP2   | 2.29                     | 0.41              |
| 26:RB:40:U:H1'    | 26:RB:45:A:N6      | 2.36                     | 0.41              |
| 27:RD:145:VAL:CG1 | 27:RD:146:GLU:N    | 2.83                     | 0.41              |
| 27:RD:147:LEU:CD1 | 27:RD:155:LEU:HD21 | 2.51                     | 0.41              |
| 27:RD:153:ALA:C   | 27:RD:154:LYS:HG3  | 2.46                     | 0.41              |
| 27:RD:263:ARG:NH1 | 27:RD:263:ARG:CB   | 2.75                     | 0.41              |
| 28:RE:4:ILE:HG22  | 28:RE:198:VAL:HB   | 2.02                     | 0.41              |
| 28:RE:51:PHE:CG   | 28:RE:52:LEU:N     | 2.89                     | 0.41              |
| 28:RE:147:PRO:HB2 | 28:RE:149:ARG:HG2  | 2.03                     | 0.41              |
| 29:RF:150:GLY:C   | 29:RF:152:GLU:H    | 2.29                     | 0.41              |
| 30:RG:95:ARG:HA   | 30:RG:99:MET:HB3   | 2.03                     | 0.41              |
| 30:RG:136:ARG:O   | 30:RG:137:GLU:C    | 2.61                     | 0.41              |
| 31:RH:145:ALA:O   | 31:RH:148:ILE:HB   | 2.21                     | 0.41              |
| 33:RN:10:GLU:OE2  | 33:RN:11:PRO:HD2   | 2.21                     | 0.41              |
| 33:RN:23:LEU:CD1  | 33:RN:99:LEU:HD23  | 2.51                     | 0.41              |
| 33:RN:56:ASN:ND2  | 33:RN:126:PRO:N    | 2.69                     | 0.41              |
| 33:RN:58:ASP:HB3  | 33:RN:95:PRO:HB3   | 2.02                     | 0.41              |
| 33:RN:137:LYS:HA  | 33:RN:137:LYS:HD2  | 1.88                     | 0.41              |
| 34:RO:111:PHE:N   | 34:RO:112:MET:HE2  | 2.36                     | 0.41              |
| 35:RP:9:ASN:HB2   | 35:RP:10:PRO:HD2   | 2.03                     | 0.41              |
| 36:RQ:139:GLU:HG2 | 36:RQ:140:ALA:N    | 2.36                     | 0.41              |
| 37:RR:55:ALA:O    | 37:RR:58:GLY:HA3   | 2.21                     | 0.41              |
| 37:RR:94:TYR:N    | 37:RR:94:TYR:CD2   | 2.87                     | 0.41              |
| 38:RS:15:ARG:O    | 38:RS:19:LYS:HD3   | 2.20                     | 0.41              |
| 38:RS:66:ALA:HA   | 38:RS:69:VAL:CG1   | 2.51                     | 0.41              |
| 39:RT:39:ARG:HG2  | 39:RT:40:THR:N     | 2.25                     | 0.41              |
| 39:RT:67:SER:O    | 39:RT:68:TYR:C     | 2.63                     | 0.41              |
| 39:RT:77:PRO:C    | 39:RT:79:HIS:H     | 2.29                     | 0.41              |
| 40:RU:57:PHE:O    | 40:RU:60:LEU:N     | 2.54                     | 0.41              |
| 40:RU:83:LEU:CD1  | 40:RU:113:ALA:HB2  | 2.50                     | 0.41              |
| 42:RW:14:PRO:HG3  | 42:RW:101:SER:OG   | 2.21                     | 0.41              |
| 42:RW:17:VAL:C    | 42:RW:19:LEU:N     | 2.76                     | 0.41              |
| 44:RY:43:ASN:O    | 44:RY:43:ASN:OD1   | 2.39                     | 0.41              |
| 46:R0:10:THR:HG22 | 46:R0:12:ASN:N     | 2.36                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 47:R1:63:ALA:C    | 47:R1:65:SER:N      | 2.78                     | 0.41              |
| 48:R2:27:GLU:CD   | 48:R2:27:GLU:H      | 2.17                     | 0.41              |
| 48:R2:48:HIS:C    | 48:R2:50:ILE:N      | 2.76                     | 0.41              |
| 50:R4:48:ARG:O    | 50:R4:49:PHE:C      | 2.63                     | 0.41              |
| 53:R7:8:ASN:OD1   | 53:R7:8:ASN:C       | 2.64                     | 0.41              |
| 54:R8:3:LYS:HE2   | 54:R8:3:LYS:HB3     | 1.82                     | 0.41              |
| 54:R8:64:TYR:HB3  | 54:R8:65:GLU:H      | 1.40                     | 0.41              |
| 1:XA:124:G:C5     | 1:XA:125:U:C4       | 3.09                     | 0.41              |
| 1:XA:575:G:H4'    | 1:XA:576:G:C5'      | 2.51                     | 0.41              |
| 1:XA:752:G:HO2'   | 1:XA:753:A:P        | 2.43                     | 0.41              |
| 1:XA:945:G:C2     | 1:XA:946:A:C8       | 3.09                     | 0.41              |
| 1:XA:1304:G:C6    | 1:XA:1305:G:C2      | 3.08                     | 0.41              |
| 1:XA:1362:C:H2'   | 1:XA:1362(A):C:H5'' | 2.02                     | 0.41              |
| 1:XA:1372:U:OP1   | 9:XI:71:SER:HB3     | 2.21                     | 0.41              |
| 2:XB:87:ARG:HH11  | 2:XB:223:ILE:HD11   | 1.82                     | 0.41              |
| 2:XB:95:GLN:HB3   | 2:XB:148:TYR:HD1    | 1.84                     | 0.41              |
| 2:XB:212:GLN:NE2  | 2:XB:212:GLN:O      | 2.54                     | 0.41              |
| 2:XB:213:LEU:C    | 2:XB:213:LEU:HD23   | 2.46                     | 0.41              |
| 3:XC:5:ILE:CD1    | 3:XC:5:ILE:H        | 2.34                     | 0.41              |
| 3:XC:47:LEU:CD1   | 3:XC:76:VAL:HG12    | 2.42                     | 0.41              |
| 4:XD:14:ARG:HD3   | 4:XD:14:ARG:C       | 2.42                     | 0.41              |
| 4:XD:165:MET:HE3  | 4:XD:165:MET:CA     | 2.44                     | 0.41              |
| 4:XD:178:VAL:HG12 | 4:XD:179:GLU:N      | 2.35                     | 0.41              |
| 6:XF:42:GLU:C     | 6:XF:44:GLY:H       | 2.29                     | 0.41              |
| 6:XF:101:ALA:HA   | 18:XR:28:GLU:CD     | 2.45                     | 0.41              |
| 8:XH:109:ILE:HG13 | 8:XH:120:THR:HB     | 2.03                     | 0.41              |
| 9:XI:10:ARG:CG    | 9:XI:105:ASP:HB2    | 2.51                     | 0.41              |
| 9:XI:83:ARG:HG2   | 9:XI:83:ARG:H       | 1.64                     | 0.41              |
| 9:XI:85:LEU:HD12  | 9:XI:85:LEU:C       | 2.45                     | 0.41              |
| 10:XJ:54:PHE:CZ   | 10:XJ:55:LYS:CE     | 3.04                     | 0.41              |
| 11:XK:92:GLU:O    | 11:XK:95:ILE:N      | 2.54                     | 0.41              |
| 12:XL:22:SER:C    | 12:XL:24:VAL:N      | 2.79                     | 0.41              |
| 12:XL:62:SER:O    | 12:XL:64:TYR:N      | 2.54                     | 0.41              |
| 12:XL:90:VAL:HG12 | 12:XL:92:ASP:H      | 1.86                     | 0.41              |
| 13:XM:110:ARG:HG3 | 13:XM:110:ARG:O     | 2.20                     | 0.41              |
| 14:XN:15:LYS:O    | 14:XN:16:PHE:C      | 2.63                     | 0.41              |
| 15:XO:69:TYR:CZ   | 15:XO:73:GLU:HG3    | 2.55                     | 0.41              |
| 16:XP:8:ARG:HG2   | 16:XP:8:ARG:NH1     | 2.31                     | 0.41              |
| 17:XQ:63:ARG:HG2  | 17:XQ:64:PRO:HD2    | 2.03                     | 0.41              |
| 17:XQ:85:VAL:HG12 | 17:XQ:85:VAL:O      | 2.20                     | 0.41              |
| 20:XT:28:ALA:O    | 20:XT:29:LYS:C      | 2.64                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:XV:16:C:O2'     | 22:XV:17:C:OP1     | 2.39                     | 0.41              |
| 25:YA:137(A):G:H1' | 43:YX:41:ASN:ND2   | 2.36                     | 0.41              |
| 25:YA:177:G:N3     | 25:YA:177:G:H5''   | 2.36                     | 0.41              |
| 25:YA:483:A:H4'    | 44:YY:49:VAL:CA    | 2.39                     | 0.41              |
| 25:YA:571:A:O2'    | 25:YA:573:G:O5'    | 2.34                     | 0.41              |
| 25:YA:603:A:N1     | 25:YA:625:G:O2'    | 2.45                     | 0.41              |
| 25:YA:812:C:H1'    | 25:YA:1250:G:C2    | 2.56                     | 0.41              |
| 25:YA:901:A:H2'    | 25:YA:901:A:N3     | 2.36                     | 0.41              |
| 25:YA:963:U:H2'    | 25:YA:964:C:C6     | 2.56                     | 0.41              |
| 25:YA:1003:G:N2    | 25:YA:1153:C:C2    | 2.88                     | 0.41              |
| 25:YA:1061:U:H5'   | 25:YA:1070:A:O2'   | 2.21                     | 0.41              |
| 25:YA:1257:C:H5'   | 29:YF:75:HIS:CE1   | 2.56                     | 0.41              |
| 25:YA:1870:C:H2'   | 25:YA:1871:A:O4'   | 2.21                     | 0.41              |
| 25:YA:2224:G:H4'   | 25:YA:2226:C:C2    | 2.56                     | 0.41              |
| 25:YA:2335:A:OP2   | 38:YS:13:ARG:HB2   | 2.20                     | 0.41              |
| 25:YA:2474:C:H3'   | 25:YA:2475:C:C6    | 2.56                     | 0.41              |
| 25:YA:2476:A:H2'   | 25:YA:2477:C:C6    | 2.55                     | 0.41              |
| 25:YA:2566:A:H4'   | 25:YA:2567:G:O5'   | 2.21                     | 0.41              |
| 25:YA:2592:G:C6    | 25:YA:2593:U:N3    | 2.89                     | 0.41              |
| 25:YA:2630:G:H2'   | 25:YA:2631:G:H8    | 1.86                     | 0.41              |
| 25:YA:2636:U:H1'   | 25:YA:2783:G:H22   | 1.86                     | 0.41              |
| 25:YA:2842:G:O2'   | 25:YA:2843:G:H5'   | 2.21                     | 0.41              |
| 27:YD:68:LYS:O     | 27:YD:68:LYS:HG3   | 2.20                     | 0.41              |
| 27:YD:98:VAL:C     | 27:YD:100:GLY:N    | 2.79                     | 0.41              |
| 27:YD:147:LEU:CD1  | 27:YD:155:LEU:HD21 | 2.51                     | 0.41              |
| 27:YD:228:PRO:HD3  | 27:YD:234:GLY:O    | 2.21                     | 0.41              |
| 28:YE:93:VAL:H     | 28:YE:95:ILE:CD1   | 2.22                     | 0.41              |
| 28:YE:134:ILE:C    | 28:YE:134:ILE:CD1  | 2.94                     | 0.41              |
| 29:YF:28:ILE:HD12  | 29:YF:28:ILE:C     | 2.46                     | 0.41              |
| 29:YF:68:LYS:O     | 29:YF:69:HIS:HB2   | 2.21                     | 0.41              |
| 29:YF:198:ALA:HA   | 29:YF:201:VAL:CG1  | 2.41                     | 0.41              |
| 30:YG:18:GLU:HA    | 30:YG:18:GLU:OE2   | 2.21                     | 0.41              |
| 30:YG:67:LYS:NZ    | 50:Y4:6:HIS:CD2    | 2.89                     | 0.41              |
| 31:YH:65:HIS:O     | 31:YH:66:GLY:C     | 2.63                     | 0.41              |
| 31:YH:145:ALA:O    | 31:YH:148:ILE:HB   | 2.21                     | 0.41              |
| 32:YI:56:LYS:HG3   | 32:YI:57:ARG:N     | 2.36                     | 0.41              |
| 33:YN:1:MET:O      | 33:YN:1:MET:HG3    | 2.19                     | 0.41              |
| 34:YO:10:VAL:HG21  | 34:YO:16:ALA:HB3   | 2.03                     | 0.41              |
| 35:YP:101:VAL:O    | 35:YP:103:ALA:N    | 2.53                     | 0.41              |
| 37:YR:29:LEU:HD11  | 37:YR:48:VAL:CG1   | 2.50                     | 0.41              |
| 37:YR:55:ALA:O     | 37:YR:58:GLY:HA3   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:YR:61:HIS:CE1  | 37:YR:65:LEU:HD11 | 2.56                     | 0.41              |
| 38:YS:88:ASP:CG   | 38:YS:89:ARG:H    | 2.28                     | 0.41              |
| 38:YS:93:LYS:HE3  | 38:YS:93:LYS:HB2  | 1.93                     | 0.41              |
| 39:YT:39:ARG:HG2  | 39:YT:40:THR:N    | 2.25                     | 0.41              |
| 40:YU:57:PHE:O    | 40:YU:60:LEU:N    | 2.54                     | 0.41              |
| 40:YU:89:GLU:C    | 40:YU:90:VAL:O    | 2.62                     | 0.41              |
| 40:YU:91:ASP:OD2  | 40:YU:96:ALA:CA   | 2.69                     | 0.41              |
| 40:YU:92:ARG:O    | 40:YU:92:ARG:CG   | 2.54                     | 0.41              |
| 42:YW:1:MET:CB    | 42:YW:64:MET:HE3  | 2.48                     | 0.41              |
| 42:YW:28:SER:C    | 42:YW:30:GLU:H    | 2.28                     | 0.41              |
| 43:YX:31:HIS:HA   | 43:YX:32:PRO:HD3  | 1.88                     | 0.41              |
| 43:YX:60:ARG:HA   | 43:YX:75:ASP:OD2  | 2.20                     | 0.41              |
| 44:YY:5:MET:CE    | 44:YY:32:PRO:HB3  | 2.51                     | 0.41              |
| 44:YY:13:VAL:O    | 44:YY:24:VAL:HA   | 2.20                     | 0.41              |
| 47:Y1:91:LYS:HG3  | 47:Y1:92:LYS:N    | 2.32                     | 0.41              |
| 48:Y2:41:ILE:HD12 | 48:Y2:43:GLN:N    | 2.35                     | 0.41              |
| 48:Y2:53:LEU:O    | 48:Y2:57:ILE:HG13 | 2.21                     | 0.41              |
| 48:Y2:61:LEU:HD23 | 48:Y2:61:LEU:HA   | 1.85                     | 0.41              |
| 50:Y4:60:GLN:HB3  | 50:Y4:61:ARG:H    | 1.56                     | 0.41              |
| 50:Y4:63:TYR:O    | 50:Y4:65:ASP:N    | 2.53                     | 0.41              |
| 52:Y6:6:ARG:HA    | 52:Y6:6:ARG:NE    | 2.35                     | 0.41              |
| 52:Y6:8:LYS:O     | 52:Y6:9:LEU:HB2   | 2.21                     | 0.41              |
| 53:Y7:8:ASN:OD1   | 53:Y7:8:ASN:C     | 2.64                     | 0.41              |
| 53:Y7:24:THR:HB   | 53:Y7:25:PRO:HD2  | 2.03                     | 0.41              |
| 54:Y8:53:PRO:C    | 54:Y8:55:ALA:N    | 2.76                     | 0.41              |
| 55:Y9:2:LYS:HD2   | 55:Y9:2:LYS:HA    | 1.96                     | 0.41              |
| 1:QA:181:G:O2'    | 1:QA:182:U:P      | 2.79                     | 0.41              |
| 1:QA:1059:C:H2'   | 1:QA:1060:C:H6    | 1.85                     | 0.41              |
| 1:QA:1124:G:OP2   | 1:QA:1124:G:H8    | 2.03                     | 0.41              |
| 2:QB:71:VAL:HG23  | 2:QB:164:VAL:HG22 | 2.02                     | 0.41              |
| 3:QC:23:TYR:CD2   | 3:QC:24:ALA:N     | 2.88                     | 0.41              |
| 3:QC:92:ALA:HB2   | 3:QC:99:VAL:HG13  | 2.03                     | 0.41              |
| 3:QC:178:LEU:N    | 3:QC:178:LEU:CD2  | 2.84                     | 0.41              |
| 4:QD:14:ARG:HA    | 4:QD:14:ARG:HD3   | 1.89                     | 0.41              |
| 4:QD:202:LEU:C    | 4:QD:204:ILE:N    | 2.78                     | 0.41              |
| 5:QE:27:ARG:CG    | 5:QE:28:PHE:N     | 2.84                     | 0.41              |
| 5:QE:41:VAL:O     | 5:QE:66:MET:HA    | 2.21                     | 0.41              |
| 5:QE:64:ARG:CZ    | 5:QE:64:ARG:HB2   | 2.51                     | 0.41              |
| 5:QE:101:ILE:HD13 | 5:QE:118:ILE:O    | 2.21                     | 0.41              |
| 7:QG:96:GLN:O     | 7:QG:97:GLN:C     | 2.61                     | 0.41              |
| 8:QH:133:LEU:C    | 8:QH:133:LEU:HD23 | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:QI:49:PRO:O      | 9:QI:85:LEU:HD21   | 2.20                     | 0.41              |
| 10:QJ:84:GLN:H     | 10:QJ:84:GLN:HG3   | 1.50                     | 0.41              |
| 12:QL:43:VAL:HG13  | 12:QL:55:VAL:HG21  | 2.03                     | 0.41              |
| 15:QO:3:ILE:H      | 15:QO:3:ILE:CD1    | 2.20                     | 0.41              |
| 15:QO:50:HIS:O     | 15:QO:53:HIS:HB3   | 2.20                     | 0.41              |
| 17:QQ:67:LYS:O     | 17:QQ:68:ARG:HB3   | 2.21                     | 0.41              |
| 18:QR:64:ARG:C     | 18:QR:66:LEU:N     | 2.79                     | 0.41              |
| 20:QT:44:ALA:HB3   | 20:QT:91:LEU:HD12  | 2.03                     | 0.41              |
| 22:QV:16:C:O2'     | 22:QV:17:C:OP1     | 2.39                     | 0.41              |
| 25:RA:222:A:H1'    | 25:RA:223:A:OP1    | 2.21                     | 0.41              |
| 25:RA:679:C:H2'    | 25:RA:680:G:C8     | 2.56                     | 0.41              |
| 25:RA:774:A:HO2'   | 25:RA:775:G:P      | 2.43                     | 0.41              |
| 25:RA:963:U:H2'    | 25:RA:964:C:C6     | 2.55                     | 0.41              |
| 25:RA:1030:G:OP2   | 36:RQ:128:LYS:HE2  | 2.21                     | 0.41              |
| 25:RA:1417:C:H2'   | 25:RA:1418:G:O4'   | 2.20                     | 0.41              |
| 25:RA:1608:A:H1'   | 25:RA:1610:A:OP2   | 2.20                     | 0.41              |
| 25:RA:1953:A:H5''  | 25:RA:1954:G:OP2   | 2.20                     | 0.41              |
| 25:RA:2572:A:C2    | 28:RE:144:ARG:NH2  | 2.89                     | 0.41              |
| 27:RD:31:LYS:O     | 27:RD:32:SER:O     | 2.39                     | 0.41              |
| 27:RD:177:LEU:C    | 27:RD:179:SER:N    | 2.79                     | 0.41              |
| 29:RF:13:SER:OG    | 29:RF:14:PRO:HD2   | 2.21                     | 0.41              |
| 29:RF:36:VAL:HG11  | 29:RF:183:VAL:HG11 | 2.03                     | 0.41              |
| 30:RG:7:LEU:CD2    | 30:RG:176:LEU:HD22 | 2.45                     | 0.41              |
| 30:RG:67:LYS:NZ    | 50:R4:6:HIS:CD2    | 2.89                     | 0.41              |
| 30:RG:95:ARG:CA    | 30:RG:99:MET:HB3   | 2.50                     | 0.41              |
| 35:RP:66:GLY:O     | 35:RP:67:MET:CB    | 2.63                     | 0.41              |
| 35:RP:84:ASN:HB2   | 35:RP:87:ASP:OD2   | 2.21                     | 0.41              |
| 35:RP:96:THR:O     | 35:RP:97:PRO:C     | 2.63                     | 0.41              |
| 35:RP:101:VAL:HG23 | 35:RP:106:LEU:HB3  | 2.03                     | 0.41              |
| 36:RQ:39:PRO:HA    | 36:RQ:97:VAL:O     | 2.21                     | 0.41              |
| 38:RS:6:ALA:O      | 38:RS:10:ARG:HD3   | 2.21                     | 0.41              |
| 38:RS:42:ASP:O     | 38:RS:43:GLU:CB    | 2.62                     | 0.41              |
| 42:RW:28:SER:C     | 42:RW:30:GLU:H     | 2.28                     | 0.41              |
| 45:RZ:53:ILE:HG22  | 45:RZ:71:VAL:HG22  | 2.02                     | 0.41              |
| 50:R4:42:PHE:CZ    | 50:R4:43:TYR:HB3   | 2.57                     | 0.41              |
| 50:R4:63:TYR:O     | 50:R4:65:ASP:N     | 2.54                     | 0.41              |
| 53:R7:24:THR:HB    | 53:R7:25:PRO:HD2   | 2.03                     | 0.41              |
| 1:XA:481:G:O2'     | 1:XA:482:A:O5'     | 2.39                     | 0.41              |
| 1:XA:667:G:H4'     | 15:XO:51:HIS:ND1   | 2.36                     | 0.41              |
| 1:XA:815:A:N3      | 1:XA:1527:C:O2'    | 2.48                     | 0.41              |
| 1:XA:967:C:H5''    | 1:XA:968:A:OP2     | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:973:G:H3'    | 1:XA:974:A:H5''   | 2.03                     | 0.41              |
| 1:XA:1314:C:H5    | 19:XS:4:SER:HB2   | 1.85                     | 0.41              |
| 1:XA:1316:G:H2'   | 1:XA:1317:C:H5''  | 2.03                     | 0.41              |
| 2:XB:97:TRP:O     | 2:XB:98:LEU:C     | 2.64                     | 0.41              |
| 2:XB:114:ARG:O    | 2:XB:118:LEU:HG   | 2.21                     | 0.41              |
| 4:XD:15:GLU:N     | 4:XD:15:GLU:OE1   | 2.54                     | 0.41              |
| 4:XD:110:PHE:HE2  | 4:XD:148:VAL:HG23 | 1.85                     | 0.41              |
| 5:XE:152:ARG:HD3  | 8:XH:44:PHE:CZ    | 2.57                     | 0.41              |
| 8:XH:20:TYR:CD1   | 8:XH:65:TYR:CD2   | 2.98                     | 0.41              |
| 9:XI:113:LYS:H    | 9:XI:113:LYS:CD   | 2.28                     | 0.41              |
| 12:XL:44:THR:HA   | 12:XL:45:PRO:HD3  | 1.70                     | 0.41              |
| 12:XL:117:ARG:HB3 | 12:XL:122:THR:HB  | 2.02                     | 0.41              |
| 13:XM:117:VAL:CG2 | 13:XM:118:ALA:H   | 2.31                     | 0.41              |
| 14:XN:48:ALA:O    | 14:XN:51:GLY:N    | 2.53                     | 0.41              |
| 18:XR:30:ASP:C    | 18:XR:32:ARG:N    | 2.79                     | 0.41              |
| 19:XS:10:PHE:CD2  | 19:XS:11:VAL:N    | 2.89                     | 0.41              |
| 20:XT:47:GLY:C    | 20:XT:49:ALA:N    | 2.72                     | 0.41              |
| 22:XV:23:C:H2'    | 22:XV:24:U:C6     | 2.55                     | 0.41              |
| 23:XY:40:G:C2'    | 23:XY:41:A:H5'    | 2.50                     | 0.41              |
| 25:YA:1063:G:H22  | 25:YA:1076:C:H1'  | 1.86                     | 0.41              |
| 25:YA:1396:U:O2   | 25:YA:1396:U:H2'  | 2.20                     | 0.41              |
| 25:YA:1706:U:O2   | 25:YA:1757:U:H5'  | 2.20                     | 0.41              |
| 25:YA:1794:U:H2'  | 25:YA:1795:C:C6   | 2.55                     | 0.41              |
| 25:YA:1930:G:N2   | 25:YA:1969:A:OP2  | 2.47                     | 0.41              |
| 25:YA:2151:G:H2'  | 25:YA:2152:G:H8   | 1.86                     | 0.41              |
| 25:YA:2283:C:H2'  | 25:YA:2284:C:O4'  | 2.21                     | 0.41              |
| 25:YA:2306:C:N4   | 30:YG:42:GLY:O    | 2.52                     | 0.41              |
| 25:YA:2467:C:O2   | 36:YQ:124:LYS:NZ  | 2.51                     | 0.41              |
| 28:YE:119:ARG:HG2 | 28:YE:160:TYR:HB2 | 2.03                     | 0.41              |
| 29:YF:59:TYR:HB3  | 29:YF:60:SER:H    | 1.70                     | 0.41              |
| 29:YF:118:ALA:HA  | 29:YF:123:LEU:HB3 | 2.02                     | 0.41              |
| 30:YG:53:LEU:CD1  | 30:YG:87:PRO:HB2  | 2.51                     | 0.41              |
| 31:YH:45:VAL:O    | 31:YH:45:VAL:CG1  | 2.69                     | 0.41              |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:CE  | 2.51                     | 0.41              |
| 31:YH:146:ALA:HA  | 31:YH:164:TYR:OH  | 2.21                     | 0.41              |
| 33:YN:61:ARG:C    | 33:YN:62:VAL:CG2  | 2.93                     | 0.41              |
| 33:YN:101:HIS:HD2 | 33:YN:102:ALA:N   | 2.19                     | 0.41              |
| 35:YP:18:ARG:HD2  | 35:YP:27:HIS:CD2  | 2.56                     | 0.41              |
| 36:YQ:20:ALA:HB1  | 36:YQ:99:PRO:CG   | 2.50                     | 0.41              |
| 36:YQ:139:GLU:CD  | 36:YQ:139:GLU:H   | 2.28                     | 0.41              |
| 41:YV:38:LEU:CD1  | 41:YV:55:ALA:CB   | 2.99                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:YW:71:VAL:HA   | 42:YW:107:LEU:HD12 | 2.02                     | 0.41              |
| 48:Y2:11:GLU:HA   | 48:Y2:14:ARG:HD2   | 2.02                     | 0.41              |
| 49:Y3:15:TYR:O    | 49:Y3:16:PRO:C     | 2.64                     | 0.41              |
| 54:Y8:17:THR:O    | 54:Y8:20:GLY:N     | 2.47                     | 0.41              |
| 54:Y8:40:GLU:O    | 54:Y8:42:ARG:N     | 2.54                     | 0.41              |
| 1:QA:134:A:H61    | 16:QP:25:ARG:NH1   | 2.19                     | 0.40              |
| 1:QA:427:U:OP2    | 1:QA:428:G:O2'     | 2.37                     | 0.40              |
| 1:QA:653:A:N7     | 8:QH:56:LYS:HB3    | 2.36                     | 0.40              |
| 1:QA:760:G:H2'    | 1:QA:761:G:O4'     | 2.21                     | 0.40              |
| 1:QA:1064:G:H1'   | 1:QA:1066:C:C6     | 2.57                     | 0.40              |
| 1:QA:1113:C:H2'   | 1:QA:1114:C:H6     | 1.85                     | 0.40              |
| 1:QA:1132:C:H2'   | 1:QA:1133:G:H8     | 1.87                     | 0.40              |
| 2:QB:86:GLU:C     | 2:QB:88:ALA:N      | 2.77                     | 0.40              |
| 2:QB:130:ARG:HH22 | 2:QB:138:LEU:HD21  | 1.85                     | 0.40              |
| 2:QB:143:GLU:O    | 2:QB:147:LYS:HB2   | 2.21                     | 0.40              |
| 3:QC:59:ARG:NH1   | 3:QC:97:LYS:HE3    | 2.34                     | 0.40              |
| 4:QD:29:PRO:HD2   | 4:QD:30:LYS:HE2    | 2.03                     | 0.40              |
| 4:QD:110:PHE:HE2  | 4:QD:148:VAL:HG23  | 1.86                     | 0.40              |
| 5:QE:6:PHE:HB2    | 5:QE:63:ARG:HH12   | 1.86                     | 0.40              |
| 5:QE:31:LEU:HD22  | 5:QE:31:LEU:HA     | 1.86                     | 0.40              |
| 8:QH:18:ARG:HA    | 8:QH:18:ARG:HD2    | 1.92                     | 0.40              |
| 10:QJ:8:LEU:HD11  | 10:QJ:23:ILE:CD1   | 2.37                     | 0.40              |
| 11:QK:25:TYR:H    | 11:QK:25:TYR:HD1   | 1.69                     | 0.40              |
| 11:QK:83:ILE:HG12 | 11:QK:109:VAL:CG2  | 2.51                     | 0.40              |
| 12:QL:22:SER:C    | 12:QL:24:VAL:N     | 2.79                     | 0.40              |
| 13:QM:36:LYS:HE3  | 13:QM:59:TYR:CD1   | 2.57                     | 0.40              |
| 16:QP:20:VAL:HG22 | 16:QP:21:VAL:H     | 1.83                     | 0.40              |
| 16:QP:59:TRP:O    | 16:QP:60:LEU:C     | 2.63                     | 0.40              |
| 17:QQ:11:VAL:HG23 | 17:QQ:12:SER:H     | 1.85                     | 0.40              |
| 19:QS:32:LYS:HA   | 19:QS:50:ALA:HB3   | 2.03                     | 0.40              |
| 23:QY:40:G:C2'    | 23:QY:41:A:H5'     | 2.51                     | 0.40              |
| 25:RA:67:U:H3     | 25:RA:74:A:H2      | 1.67                     | 0.40              |
| 25:RA:83:G:H1     | 25:RA:102:G:H1'    | 1.87                     | 0.40              |
| 25:RA:686:G:O6    | 53:R7:12:ARG:HG3   | 2.21                     | 0.40              |
| 25:RA:1062:G:N3   | 25:RA:1077:A:N6    | 2.69                     | 0.40              |
| 25:RA:1208:C:C4   | 25:RA:1209:G:N7    | 2.89                     | 0.40              |
| 25:RA:1300:U:H4'  | 25:RA:1301:A:H5''  | 2.04                     | 0.40              |
| 25:RA:1355:G:C4   | 25:RA:1356:G:C8    | 3.09                     | 0.40              |
| 25:RA:1459:G:H2'  | 25:RA:1460:A:H5''  | 2.02                     | 0.40              |
| 25:RA:1543:A:H1'  | 25:RA:1545:A:O4'   | 2.20                     | 0.40              |
| 25:RA:1870:C:H2'  | 25:RA:1871:A:O4'   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2776:A:H4'  | 25:RA:2777:G:O5'   | 2.22                     | 0.40              |
| 27:RD:272:ALA:HB1 | 27:RD:273:ARG:H    | 1.58                     | 0.40              |
| 28:RE:70:ALA:O    | 28:RE:71:GLY:C     | 2.62                     | 0.40              |
| 29:RF:128:ALA:O   | 29:RF:129:PHE:CB   | 2.67                     | 0.40              |
| 32:RI:8:PRO:HG3   | 32:RI:14:ASP:HB2   | 2.03                     | 0.40              |
| 34:RO:20:MET:O    | 34:RO:41:ALA:CB    | 2.67                     | 0.40              |
| 36:RQ:66:ILE:O    | 36:RQ:67:ARG:HB2   | 2.22                     | 0.40              |
| 37:RR:22:ARG:O    | 37:RR:26:LYS:HG3   | 2.21                     | 0.40              |
| 38:RS:106:ARG:HB2 | 38:RS:106:ARG:CZ   | 2.49                     | 0.40              |
| 40:RU:78:THR:O    | 40:RU:79:PHE:C     | 2.64                     | 0.40              |
| 45:RZ:144:LEU:HG  | 45:RZ:150:LEU:HD12 | 2.03                     | 0.40              |
| 45:RZ:166:SER:H   | 45:RZ:167:PRO:HA   | 1.86                     | 0.40              |
| 50:R4:26:SER:O    | 50:R4:27:THR:O     | 2.39                     | 0.40              |
| 53:R7:5:TRP:HE1   | 53:R7:7:PRO:HG3    | 1.85                     | 0.40              |
| 1:XA:160:A:H2'    | 1:XA:161:A:O4'     | 2.21                     | 0.40              |
| 1:XA:918:A:H2'    | 1:XA:919:A:H8      | 1.86                     | 0.40              |
| 1:XA:963:G:H21    | 10:XJ:55:LYS:CE    | 2.34                     | 0.40              |
| 2:XB:76:GLN:OE1   | 2:XB:206:ASP:HB3   | 2.21                     | 0.40              |
| 2:XB:132:LYS:HA   | 2:XB:135:GLN:CG    | 2.51                     | 0.40              |
| 2:XB:223:ILE:O    | 2:XB:226:ARG:HB3   | 2.20                     | 0.40              |
| 3:XC:47:LEU:HD11  | 3:XC:76:VAL:CG1    | 2.42                     | 0.40              |
| 3:XC:138:VAL:HG22 | 3:XC:151:VAL:HG23  | 2.03                     | 0.40              |
| 4:XD:19:LEU:HG    | 4:XD:21:LEU:HG     | 2.03                     | 0.40              |
| 4:XD:68:TYR:OH    | 4:XD:196:LEU:HD21  | 2.21                     | 0.40              |
| 5:XE:6:PHE:HB2    | 5:XE:63:ARG:HH12   | 1.86                     | 0.40              |
| 7:XG:21:VAL:HG23  | 7:XG:22:LEU:N      | 2.32                     | 0.40              |
| 7:XG:92:SER:HB3   | 7:XG:95:ARG:HB2    | 2.03                     | 0.40              |
| 7:XG:118:VAL:HG23 | 7:XG:119:ARG:N     | 2.35                     | 0.40              |
| 7:XG:121:ALA:O    | 7:XG:125:MET:HG3   | 2.20                     | 0.40              |
| 8:XH:33:GLU:O     | 8:XH:36:LEU:N      | 2.53                     | 0.40              |
| 9:XI:9:ARG:CG     | 9:XI:14:VAL:HG22   | 2.51                     | 0.40              |
| 10:XJ:84:GLN:H    | 10:XJ:84:GLN:HG3   | 1.50                     | 0.40              |
| 12:XL:43:VAL:HG13 | 12:XL:55:VAL:HG21  | 2.03                     | 0.40              |
| 14:XN:47:LEU:O    | 14:XN:50:LYS:N     | 2.52                     | 0.40              |
| 16:XP:50:LYS:HD3  | 16:XP:51:VAL:O     | 2.21                     | 0.40              |
| 17:XQ:94:ASN:O    | 17:XQ:97:SER:N     | 2.53                     | 0.40              |
| 18:XR:37:VAL:O    | 18:XR:40:LEU:N     | 2.54                     | 0.40              |
| 19:XS:31:ILE:HG23 | 19:XS:31:ILE:O     | 2.21                     | 0.40              |
| 20:XT:50:GLU:HA   | 20:XT:100:ILE:HG22 | 2.02                     | 0.40              |
| 20:XT:97:ALA:C    | 20:XT:99:LEU:HD13  | 2.46                     | 0.40              |
| 25:YA:263:C:H2'   | 25:YA:264:C:O4'    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:568:U:O2'   | 25:YA:570:G:N7    | 2.47                     | 0.40              |
| 25:YA:675:A:N3    | 25:YA:2443:C:O2'  | 2.53                     | 0.40              |
| 25:YA:1053:C:H42  | 25:YA:1106:G:H1   | 1.69                     | 0.40              |
| 25:YA:1268:A:H2'  | 25:YA:1269:A:O4'  | 2.21                     | 0.40              |
| 25:YA:1690:A:H2'  | 25:YA:1691:C:O4'  | 2.21                     | 0.40              |
| 25:YA:2046:G:H2'  | 25:YA:2047:U:C6   | 2.57                     | 0.40              |
| 25:YA:2072:G:H2'  | 25:YA:2073:C:C6   | 2.57                     | 0.40              |
| 25:YA:2216:G:H2'  | 25:YA:2217:G:H8   | 1.85                     | 0.40              |
| 25:YA:2310:A:H61  | 30:YG:79:ASN:HB2  | 1.86                     | 0.40              |
| 25:YA:2328:A:H2'  | 25:YA:2329:G:C8   | 2.56                     | 0.40              |
| 25:YA:2489:G:C5   | 25:YA:2490:G:C6   | 3.09                     | 0.40              |
| 25:YA:2699:C:H2'  | 25:YA:2700:C:O4'  | 2.21                     | 0.40              |
| 25:YA:2803:C:H2'  | 25:YA:2804:C:C6   | 2.56                     | 0.40              |
| 27:YD:31:LYS:O    | 27:YD:32:SER:O    | 2.39                     | 0.40              |
| 28:YE:71:GLY:O    | 28:YE:72:VAL:C    | 2.63                     | 0.40              |
| 30:YG:34:LEU:HD11 | 30:YG:99:MET:CE   | 2.49                     | 0.40              |
| 33:YN:10:GLU:OE2  | 33:YN:11:PRO:HD2  | 2.21                     | 0.40              |
| 34:YO:16:ALA:HA   | 34:YO:46:ALA:CB   | 2.50                     | 0.40              |
| 34:YO:111:PHE:N   | 34:YO:112:MET:HE2 | 2.36                     | 0.40              |
| 35:YP:84:ASN:HB2  | 35:YP:87:ASP:OD2  | 2.22                     | 0.40              |
| 35:YP:85:LEU:HA   | 35:YP:85:LEU:HD23 | 1.92                     | 0.40              |
| 36:YQ:139:GLU:CG  | 36:YQ:140:ALA:N   | 2.84                     | 0.40              |
| 38:YS:20:ARG:HE   | 38:YS:21:THR:HA   | 1.87                     | 0.40              |
| 38:YS:61:ASN:OD1  | 38:YS:63:THR:OG1  | 2.29                     | 0.40              |
| 42:YW:66:GLU:HG2  | 42:YW:67:ASP:N    | 2.37                     | 0.40              |
| 44:YY:14:LEU:HD23 | 44:YY:14:LEU:C    | 2.46                     | 0.40              |
| 44:YY:42:VAL:HG21 | 44:YY:67:LEU:CD1  | 2.52                     | 0.40              |
| 44:YY:97:ARG:NH2  | 44:YY:98:VAL:CG2  | 2.85                     | 0.40              |
| 47:Y1:85:LEU:N    | 47:Y1:85:LEU:CD2  | 2.84                     | 0.40              |
| 47:Y1:94:LEU:HD23 | 47:Y1:94:LEU:HA   | 1.82                     | 0.40              |
| 54:Y8:38:GLY:C    | 54:Y8:40:GLU:N    | 2.79                     | 0.40              |
| 1:QA:114:U:H2'    | 1:QA:115:G:C8     | 2.56                     | 0.40              |
| 1:QA:236:G:OP1    | 17:QQ:40:LYS:NZ   | 2.44                     | 0.40              |
| 1:QA:412:A:H1'    | 1:QA:413:G:OP2    | 2.21                     | 0.40              |
| 1:QA:578:C:O2'    | 1:QA:728:A:N3     | 2.52                     | 0.40              |
| 1:QA:1410:G:H2'   | 1:QA:1411:C:H6    | 1.85                     | 0.40              |
| 1:QA:1508:G:H2'   | 1:QA:1509:C:C6    | 2.56                     | 0.40              |
| 2:QB:17:PHE:HB2   | 2:QB:42:ILE:CG2   | 2.50                     | 0.40              |
| 2:QB:212:GLN:NE2  | 2:QB:212:GLN:O    | 2.54                     | 0.40              |
| 3:QC:140:ARG:HB2  | 3:QC:140:ARG:NH1  | 2.36                     | 0.40              |
| 4:QD:129:ASN:CA   | 4:QD:145:GLU:HB2  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:QF:53:ALA:C     | 6:QF:55:ASP:N      | 2.79                     | 0.40              |
| 7:QG:87:VAL:HG11  | 7:QG:155:ARG:HA    | 2.03                     | 0.40              |
| 8:QH:100:ILE:HA   | 8:QH:101:PRO:HD3   | 1.85                     | 0.40              |
| 10:QJ:65:LEU:HA   | 14:QN:55:GLY:O     | 2.21                     | 0.40              |
| 10:QJ:101:VAL:O   | 10:QJ:101:VAL:HG13 | 2.22                     | 0.40              |
| 11:QK:105:VAL:C   | 11:QK:107:SER:H    | 2.30                     | 0.40              |
| 12:QL:45:PRO:C    | 12:QL:46:LYS:O     | 2.63                     | 0.40              |
| 14:QN:34:TYR:CD1  | 14:QN:34:TYR:N     | 2.89                     | 0.40              |
| 19:QS:31:ILE:HG23 | 19:QS:31:ILE:O     | 2.21                     | 0.40              |
| 25:RA:320:A:H4'   | 25:RA:322:A:C8     | 2.56                     | 0.40              |
| 25:RA:1680:U:O2'  | 25:RA:1763:G:N7    | 2.52                     | 0.40              |
| 25:RA:1930:G:O2'  | 25:RA:1931:U:P     | 2.79                     | 0.40              |
| 25:RA:2102:U:H2'  | 25:RA:2103:C:C6    | 2.56                     | 0.40              |
| 25:RA:2105:C:H2'  | 25:RA:2106:G:H8    | 1.86                     | 0.40              |
| 25:RA:2123:G:H2'  | 25:RA:2124:G:C8    | 2.53                     | 0.40              |
| 25:RA:2674:G:H2'  | 25:RA:2675:A:C8    | 2.57                     | 0.40              |
| 26:RB:44:G:H1'    | 26:RB:47:C:N4      | 2.35                     | 0.40              |
| 28:RE:65:GLY:O    | 28:RE:66:HIS:C     | 2.64                     | 0.40              |
| 28:RE:161:GLY:O   | 28:RE:162:ALA:HB3  | 2.21                     | 0.40              |
| 29:RF:62:ARG:HB3  | 29:RF:62:ARG:CZ    | 2.51                     | 0.40              |
| 29:RF:68:LYS:O    | 29:RF:69:HIS:HB2   | 2.21                     | 0.40              |
| 29:RF:80:ALA:O    | 29:RF:83:PHE:HB2   | 2.20                     | 0.40              |
| 31:RH:65:HIS:O    | 31:RH:66:GLY:C     | 2.63                     | 0.40              |
| 33:RN:61:ARG:C    | 33:RN:62:VAL:CG2   | 2.94                     | 0.40              |
| 36:RQ:76:LYS:HB3  | 36:RQ:90:VAL:CG1   | 2.51                     | 0.40              |
| 36:RQ:108:GLY:CA  | 45:RZ:116:VAL:HG11 | 2.51                     | 0.40              |
| 38:RS:61:ASN:OD1  | 38:RS:63:THR:OG1   | 2.29                     | 0.40              |
| 38:RS:100:ALA:CA  | 38:RS:103:GLU:HG2  | 2.49                     | 0.40              |
| 41:RV:38:LEU:O    | 41:RV:51:VAL:HA    | 2.21                     | 0.40              |
| 41:RV:55:ALA:O    | 41:RV:56:SER:OG    | 2.31                     | 0.40              |
| 45:RZ:5:LEU:O     | 45:RZ:6:LYS:HB2    | 2.21                     | 0.40              |
| 45:RZ:111:VAL:O   | 45:RZ:113:ALA:N    | 2.54                     | 0.40              |
| 47:R1:85:LEU:N    | 47:R1:85:LEU:CD2   | 2.84                     | 0.40              |
| 47:R1:96:LYS:O    | 47:R1:96:LYS:HG2   | 2.21                     | 0.40              |
| 48:R2:32:LEU:O    | 48:R2:32:LEU:HD23  | 2.22                     | 0.40              |
| 54:R8:32:LEU:HD23 | 54:R8:32:LEU:HA    | 1.94                     | 0.40              |
| 54:R8:53:PRO:HD2  | 54:R8:54:GLU:H     | 1.84                     | 0.40              |
| 54:R8:53:PRO:CG   | 54:R8:54:GLU:N     | 2.84                     | 0.40              |
| 55:R9:10:ILE:HD12 | 55:R9:32:HIS:CG    | 2.56                     | 0.40              |
| 1:XA:304:U:H2'    | 1:XA:305:G:C8      | 2.56                     | 0.40              |
| 1:XA:545:C:H2'    | 1:XA:546:G:O4'     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:595:G:H1'    | 1:XA:596:C:C5     | 2.56                     | 0.40              |
| 1:XA:884:U:H4'    | 1:XA:885:G:H5''   | 2.02                     | 0.40              |
| 1:XA:980:C:H5''   | 1:XA:981:U:C5     | 2.56                     | 0.40              |
| 1:XA:1268:A:H4'   | 21:XU:19:GLY:C    | 2.46                     | 0.40              |
| 1:XA:1279:A:OP2   | 10:XJ:9:ARG:NH1   | 2.54                     | 0.40              |
| 2:XB:17:PHE:HB2   | 2:XB:42:ILE:CG2   | 2.50                     | 0.40              |
| 2:XB:143:GLU:O    | 2:XB:147:LYS:HB2  | 2.22                     | 0.40              |
| 2:XB:168:THR:CG2  | 2:XB:192:SER:HB2  | 2.51                     | 0.40              |
| 3:XC:178:LEU:N    | 3:XC:178:LEU:CD2  | 2.85                     | 0.40              |
| 4:XD:120:LEU:CD2  | 4:XD:125:HIS:HB2  | 2.46                     | 0.40              |
| 8:XH:1:MET:O      | 8:XH:2:LEU:HB2    | 2.21                     | 0.40              |
| 9:XI:80:GLY:C     | 9:XI:82:ALA:H     | 2.29                     | 0.40              |
| 10:XJ:22:LYS:HZ1  | 10:XJ:23:ILE:HG12 | 1.86                     | 0.40              |
| 11:XK:21:ILE:CD1  | 11:XK:82:VAL:HG13 | 2.51                     | 0.40              |
| 11:XK:105:VAL:C   | 11:XK:107:SER:H   | 2.29                     | 0.40              |
| 13:XM:40:ASN:HA   | 13:XM:41:PRO:HD3  | 1.84                     | 0.40              |
| 13:XM:122:LYS:O   | 13:XM:122:LYS:HE2 | 2.21                     | 0.40              |
| 14:XN:44:LEU:HD12 | 14:XN:53:LEU:HD12 | 1.94                     | 0.40              |
| 17:XQ:68:ARG:O    | 17:XQ:68:ARG:HG3  | 2.21                     | 0.40              |
| 18:XR:73:ALA:HB3  | 18:XR:79:LEU:CD1  | 2.47                     | 0.40              |
| 22:XV:21:A:N6     | 22:XV:46:G:H2'    | 2.36                     | 0.40              |
| 25:YA:229:A:OP1   | 25:YA:229:A:H4'   | 2.17                     | 0.40              |
| 25:YA:559:G:N2    | 40:YU:49:HIS:CE1  | 2.90                     | 0.40              |
| 25:YA:1266:G:OP2  | 51:Y5:20:ARG:NE   | 2.47                     | 0.40              |
| 25:YA:2419:U:O5'  | 25:YA:2419:U:H6   | 2.04                     | 0.40              |
| 25:YA:2648:C:H2'  | 25:YA:2649:U:C6   | 2.56                     | 0.40              |
| 25:YA:2687:U:C4   | 25:YA:2688:U:C5   | 3.09                     | 0.40              |
| 25:YA:2823:A:OP1  | 28:YE:113:PHE:HB2 | 2.21                     | 0.40              |
| 25:YA:2845:G:O2'  | 25:YA:2846:G:H5'  | 2.21                     | 0.40              |
| 27:YD:13:ARG:HG2  | 27:YD:13:ARG:O    | 2.20                     | 0.40              |
| 27:YD:230:ASP:OD2 | 27:YD:230:ASP:N   | 2.54                     | 0.40              |
| 28:YE:179:GLU:C   | 28:YE:181:LEU:H   | 2.29                     | 0.40              |
| 29:YF:62:ARG:HB3  | 29:YF:62:ARG:CZ   | 2.52                     | 0.40              |
| 30:YG:61:ALA:CB   | 30:YG:67:LYS:HA   | 2.51                     | 0.40              |
| 30:YG:112:PRO:CA  | 50:Y4:37:SER:HB2  | 2.51                     | 0.40              |
| 31:YH:20:ALA:HB3  | 31:YH:23:ARG:HG2  | 2.03                     | 0.40              |
| 31:YH:26:VAL:HG12 | 31:YH:33:LEU:HB2  | 2.03                     | 0.40              |
| 33:YN:39:ARG:C    | 33:YN:41:ASP:H    | 2.28                     | 0.40              |
| 34:YO:13:ASN:HD21 | 34:YO:97:ARG:HB3  | 1.87                     | 0.40              |
| 34:YO:86:ILE:N    | 34:YO:86:ILE:CD1  | 2.83                     | 0.40              |
| 37:YR:79:LEU:C    | 37:YR:79:LEU:CD2  | 2.93                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:89:ARG:HG2   | 38:YS:89:ARG:NH1  | 2.36                     | 0.40              |
| 38:YS:99:LYS:HE2   | 38:YS:103:GLU:OE2 | 2.20                     | 0.40              |
| 39:YT:20:PRO:HG2   | 39:YT:86:ILE:O    | 2.21                     | 0.40              |
| 39:YT:29:ARG:HB2   | 39:YT:29:ARG:NH1  | 2.36                     | 0.40              |
| 39:YT:50:ILE:CG2   | 39:YT:62:THR:OG1  | 2.67                     | 0.40              |
| 40:YU:76:TYR:O     | 40:YU:80:ILE:HG12 | 2.21                     | 0.40              |
| 41:YV:35:LEU:O     | 41:YV:36:PRO:C    | 2.65                     | 0.40              |
| 45:YZ:182:LYS:CB   | 45:YZ:183:LEU:HA  | 2.50                     | 0.40              |
| 52:Y6:50:ARG:NH1   | 52:Y6:50:ARG:HG2  | 2.37                     | 0.40              |
| 54:Y8:32:LEU:HD23  | 54:Y8:32:LEU:HA   | 1.94                     | 0.40              |
| 54:Y8:64:TYR:HB3   | 54:Y8:65:GLU:H    | 1.40                     | 0.40              |
| 1:QA:377:G:P       | 16:QP:5:ARG:HH11  | 2.40                     | 0.40              |
| 1:QA:672:U:H2'     | 1:QA:673:G:H8     | 1.87                     | 0.40              |
| 1:QA:775:G:H2'     | 1:QA:776:G:O4'    | 2.21                     | 0.40              |
| 1:QA:1178:G:C8     | 1:QA:1180:A:OP2   | 2.74                     | 0.40              |
| 1:QA:1316:G:H5''   | 14:QN:17:LYS:CE   | 2.51                     | 0.40              |
| 3:QC:128:PHE:O     | 3:QC:130:VAL:N    | 2.54                     | 0.40              |
| 6:QF:42:GLU:C      | 6:QF:44:GLY:H     | 2.30                     | 0.40              |
| 8:QH:109:ILE:HG13  | 8:QH:120:THR:HB   | 2.03                     | 0.40              |
| 9:QI:13:ALA:H      | 9:QI:68:GLY:HA3   | 1.86                     | 0.40              |
| 12:QL:62:SER:C     | 12:QL:64:TYR:N    | 2.79                     | 0.40              |
| 13:QM:39:ILE:CD1   | 13:QM:56:LEU:HB2  | 2.50                     | 0.40              |
| 18:QR:37:VAL:O     | 18:QR:38:GLU:C    | 2.63                     | 0.40              |
| 18:QR:37:VAL:O     | 18:QR:40:LEU:N    | 2.54                     | 0.40              |
| 18:QR:74:ARG:HG2   | 18:QR:79:LEU:HB2  | 2.02                     | 0.40              |
| 25:RA:95:G:HO2'    | 48:R2:48:HIS:CE1  | 2.32                     | 0.40              |
| 25:RA:102:G:H4'    | 25:RA:103:A:O5'   | 2.20                     | 0.40              |
| 25:RA:447:A:O2'    | 25:RA:473:G:N7    | 2.43                     | 0.40              |
| 25:RA:527:C:H5'    | 25:RA:2779:U:C4   | 2.57                     | 0.40              |
| 25:RA:1291:C:H5'   | 25:RA:1536:A:H5'  | 2.03                     | 0.40              |
| 25:RA:2853:C:H2'   | 25:RA:2854:G:H8   | 1.86                     | 0.40              |
| 27:RD:117:VAL:HG22 | 27:RD:118:VAL:N   | 2.35                     | 0.40              |
| 27:RD:228:PRO:HD3  | 27:RD:234:GLY:O   | 2.21                     | 0.40              |
| 28:RE:119:ARG:HG2  | 28:RE:160:TYR:HB2 | 2.04                     | 0.40              |
| 30:RG:114:ILE:HG22 | 30:RG:117:PHE:HB2 | 2.01                     | 0.40              |
| 32:RI:13:GLY:HA3   | 32:RI:17:GLN:CD   | 2.46                     | 0.40              |
| 34:RO:47:ILE:HD12  | 34:RO:48:PRO:CD   | 2.43                     | 0.40              |
| 35:RP:65:ARG:HH21  | 54:R8:15:LYS:HB3  | 1.85                     | 0.40              |
| 37:RR:14:SER:HB2   | 37:RR:15:SER:H    | 1.72                     | 0.40              |
| 38:RS:12:PHE:HD2   | 38:RS:12:PHE:HA   | 1.80                     | 0.40              |
| 38:RS:24:LEU:HD22  | 38:RS:24:LEU:N    | 2.36                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:RU:25:TRP:O    | 40:RU:26:GLY:C     | 2.65                     | 0.40              |
| 42:RW:100:THR:O   | 42:RW:100:THR:HG23 | 2.22                     | 0.40              |
| 43:RX:60:ARG:HH22 | 53:R7:47:ARG:HH12  | 1.68                     | 0.40              |
| 44:RY:95:LYS:HA   | 44:RY:101:LYS:CB   | 2.51                     | 0.40              |
| 47:R1:82:LEU:HD13 | 47:R1:83:GLU:CA    | 2.49                     | 0.40              |
| 48:R2:11:GLU:HA   | 48:R2:14:ARG:HD2   | 2.03                     | 0.40              |
| 50:R4:21:VAL:O    | 50:R4:22:ILE:O     | 2.40                     | 0.40              |
| 52:R6:37:ARG:O    | 52:R6:48:VAL:O     | 2.39                     | 0.40              |
| 54:R8:40:GLU:O    | 54:R8:42:ARG:N     | 2.54                     | 0.40              |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:H8   | 1.86                     | 0.40              |
| 1:XA:694:A:H2'    | 1:XA:695:A:O4'     | 2.21                     | 0.40              |
| 1:XA:784:C:H4'    | 25:YA:1837:C:OP1   | 2.22                     | 0.40              |
| 1:XA:815:A:H4'    | 1:XA:816:A:O5'     | 2.20                     | 0.40              |
| 2:XB:70:PHE:O     | 2:XB:92:TYR:HA     | 2.22                     | 0.40              |
| 2:XB:97:TRP:CH2   | 2:XB:176:GLU:HB2   | 2.54                     | 0.40              |
| 3:XC:13:GLY:O     | 3:XC:14:ILE:HB     | 2.22                     | 0.40              |
| 3:XC:108:ASN:HB3  | 3:XC:111:LEU:CG    | 2.51                     | 0.40              |
| 3:XC:140:ARG:HB2  | 3:XC:140:ARG:NH1   | 2.36                     | 0.40              |
| 4:XD:47:ARG:O     | 4:XD:48:ALA:C      | 2.65                     | 0.40              |
| 4:XD:170:VAL:CG2  | 4:XD:171:GLY:H     | 2.17                     | 0.40              |
| 6:XF:8:ILE:HG22   | 6:XF:10:LEU:HD12   | 2.03                     | 0.40              |
| 6:XF:40:VAL:HA    | 6:XF:62:TRP:O      | 2.22                     | 0.40              |
| 13:XM:4:ILE:CG2   | 13:XM:5:ALA:H      | 2.29                     | 0.40              |
| 13:XM:20:THR:C    | 13:XM:22:ILE:H     | 2.29                     | 0.40              |
| 13:XM:54:VAL:O    | 13:XM:54:VAL:HG12  | 2.21                     | 0.40              |
| 13:XM:94:ARG:O    | 13:XM:95:GLY:C     | 2.64                     | 0.40              |
| 18:XR:84:LYS:H    | 18:XR:84:LYS:HG2   | 1.56                     | 0.40              |
| 19:XS:5:LEU:CG    | 50:Y4:66:SER:CB    | 3.00                     | 0.40              |
| 20:XT:44:ALA:HB3  | 20:XT:91:LEU:HD12  | 2.03                     | 0.40              |
| 25:YA:26:G:C6     | 25:YA:27:G:N1      | 2.89                     | 0.40              |
| 25:YA:860:U:C5    | 25:YA:917:A:H2     | 2.39                     | 0.40              |
| 25:YA:1278:A:O3'  | 37:YR:34:ILE:HG23  | 2.21                     | 0.40              |
| 25:YA:1424:G:H2'  | 25:YA:1425:G:O4'   | 2.22                     | 0.40              |
| 25:YA:1792:G:O2'  | 25:YA:1830:C:OP1   | 2.39                     | 0.40              |
| 25:YA:1824:G:OP1  | 27:YD:52:ARG:HD3   | 2.21                     | 0.40              |
| 25:YA:2630:G:H2'  | 25:YA:2631:G:C8    | 2.56                     | 0.40              |
| 27:YD:177:LEU:C   | 27:YD:179:SER:N    | 2.80                     | 0.40              |
| 28:YE:93:VAL:HG21 | 28:YE:180:ASN:HA   | 2.03                     | 0.40              |
| 29:YF:13:SER:OG   | 29:YF:14:PRO:HD2   | 2.21                     | 0.40              |
| 29:YF:33:LEU:O    | 29:YF:37:VAL:HG23  | 2.21                     | 0.40              |
| 29:YF:36:VAL:HG11 | 29:YF:183:VAL:HG11 | 2.04                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:YF:127:GLU:C    | 29:YF:129:PHE:H   | 2.26                     | 0.40              |
| 30:YG:121:ASN:C    | 30:YG:123:ASN:N   | 2.80                     | 0.40              |
| 31:YH:128:PRO:CG   | 31:YH:129:THR:H   | 2.33                     | 0.40              |
| 32:YI:78:THR:HG22  | 32:YI:141:LYS:HD2 | 2.04                     | 0.40              |
| 33:YN:7:LYS:CG     | 33:YN:8:GLN:N     | 2.81                     | 0.40              |
| 34:YO:106:LEU:HD23 | 34:YO:106:LEU:HA  | 1.89                     | 0.40              |
| 36:YQ:139:GLU:HG2  | 36:YQ:140:ALA:N   | 2.36                     | 0.40              |
| 39:YT:55:ASN:O     | 39:YT:55:ASN:CG   | 2.64                     | 0.40              |
| 41:YV:24:LYS:CA    | 41:YV:92:THR:HG23 | 2.39                     | 0.40              |
| 43:YX:15:GLU:CD    | 43:YX:15:GLU:H    | 2.27                     | 0.40              |
| 45:YZ:131:ARG:H    | 45:YZ:131:ARG:HG2 | 1.70                     | 0.40              |
| 50:Y4:21:VAL:O     | 50:Y4:22:ILE:O    | 2.40                     | 0.40              |
| 54:Y8:53:PRO:O     | 54:Y8:54:GLU:C    | 2.64                     | 0.40              |
| 1:QA:173:U:H5''    | 1:QA:197:A:O4'    | 2.21                     | 0.40              |
| 1:QA:526:C:C4      | 1:QA:527:G:H1'    | 2.57                     | 0.40              |
| 1:QA:952:U:H2'     | 1:QA:953:G:H8     | 1.86                     | 0.40              |
| 1:QA:1326:C:OP1    | 21:QU:12:LYS:HE3  | 2.21                     | 0.40              |
| 1:QA:1336:C:O2'    | 1:QA:1337:G:O5'   | 2.39                     | 0.40              |
| 2:QB:12:GLU:C      | 2:QB:14:GLY:H     | 2.28                     | 0.40              |
| 2:QB:76:GLN:OE1    | 2:QB:206:ASP:HB3  | 2.21                     | 0.40              |
| 3:QC:13:GLY:O      | 3:QC:14:ILE:HB    | 2.21                     | 0.40              |
| 3:QC:113:ALA:HB3   | 3:QC:114:PRO:CD   | 2.43                     | 0.40              |
| 3:QC:178:LEU:C     | 3:QC:180:ALA:H    | 2.30                     | 0.40              |
| 4:QD:3:ARG:HB3     | 4:QD:69:GLY:O     | 2.21                     | 0.40              |
| 4:QD:19:LEU:HG     | 4:QD:21:LEU:HG    | 2.03                     | 0.40              |
| 4:QD:52:SER:HB3    | 4:QD:55:ALA:HB3   | 2.01                     | 0.40              |
| 4:QD:101:LEU:HD12  | 4:QD:101:LEU:C    | 2.45                     | 0.40              |
| 8:QH:1:MET:O       | 8:QH:2:LEU:HB2    | 2.21                     | 0.40              |
| 8:QH:105:ARG:O     | 8:QH:107:LEU:N    | 2.47                     | 0.40              |
| 13:QM:122:LYS:HE2  | 13:QM:122:LYS:O   | 2.21                     | 0.40              |
| 14:QN:48:ALA:O     | 14:QN:51:GLY:N    | 2.53                     | 0.40              |
| 15:QO:77:ARG:CA    | 15:QO:80:ALA:HB3  | 2.51                     | 0.40              |
| 16:QP:26:ARG:HH21  | 16:QP:31:LYS:HG2  | 1.86                     | 0.40              |
| 16:QP:39:TYR:CD2   | 16:QP:41:PRO:HD3  | 2.56                     | 0.40              |
| 17:QQ:83:ASP:O     | 17:QQ:87:LYS:HG2  | 2.21                     | 0.40              |
| 25:RA:328:U:H4'    | 44:RY:68:HIS:CE1  | 2.56                     | 0.40              |
| 25:RA:729:G:H2'    | 25:RA:1775:U:H1'  | 2.03                     | 0.40              |
| 25:RA:1357:U:H2'   | 25:RA:1358:G:O4'  | 2.21                     | 0.40              |
| 25:RA:1649:G:C6    | 25:RA:2009:G:C6   | 3.10                     | 0.40              |
| 25:RA:1754:C:H5'   | 39:RT:101:PHE:CE2 | 2.57                     | 0.40              |
| 25:RA:2451:A:N3    | 56:Z6:76:PPU:HD2  | 2.37                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:RD:72:LYS:HG3  | 27:RD:97:TYR:CE2  | 2.56                     | 0.40              |
| 27:RD:92:ILE:CD1  | 27:RD:104:TYR:CD2 | 3.05                     | 0.40              |
| 27:RD:210:GLY:O   | 27:RD:211:ARG:C   | 2.64                     | 0.40              |
| 30:RG:41:GLN:HB3  | 30:RG:43:LEU:CD1  | 2.51                     | 0.40              |
| 31:RH:26:VAL:HG12 | 31:RH:33:LEU:HB2  | 2.03                     | 0.40              |
| 33:RN:101:HIS:ND1 | 33:RN:102:ALA:N   | 2.69                     | 0.40              |
| 33:RN:113:GLY:C   | 33:RN:114:ARG:O   | 2.58                     | 0.40              |
| 35:RP:19:VAL:HG22 | 35:RP:21:ARG:N    | 2.36                     | 0.40              |
| 37:RR:34:ILE:HG22 | 37:RR:35:THR:N    | 2.35                     | 0.40              |
| 38:RS:20:ARG:HE   | 38:RS:21:THR:HA   | 1.87                     | 0.40              |
| 38:RS:52:SER:HB2  | 38:RS:55:ALA:HB3  | 2.03                     | 0.40              |
| 38:RS:89:ARG:HG2  | 38:RS:89:ARG:NH1  | 2.36                     | 0.40              |
| 38:RS:92:TYR:HB2  | 38:RS:98:VAL:HG11 | 2.02                     | 0.40              |
| 39:RT:54:ARG:HA   | 39:RT:59:THR:HG23 | 2.02                     | 0.40              |
| 44:RY:90:LEU:HB2  | 44:RY:91:GLU:H    | 1.53                     | 0.40              |
| 45:RZ:35:ARG:O    | 45:RZ:37:VAL:HG13 | 2.22                     | 0.40              |
| 48:R2:53:LEU:O    | 48:R2:57:ILE:HG13 | 2.21                     | 0.40              |
| 52:R6:24:GLU:HB3  | 52:R6:25:LYS:H    | 1.56                     | 0.40              |
| 52:R6:36:LEU:CD1  | 52:R6:50:ARG:NH1  | 2.82                     | 0.40              |
| 52:R6:50:ARG:NH1  | 52:R6:50:ARG:HG2  | 2.37                     | 0.40              |
| 1:XA:129(A):G:H1' | 1:XA:190:G:H5''   | 2.03                     | 0.40              |
| 1:XA:738:C:H2'    | 1:XA:739:C:C6     | 2.56                     | 0.40              |
| 1:XA:1131:G:H1    | 1:XA:1143:G:H21   | 1.70                     | 0.40              |
| 1:XA:1329:A:P     | 13:XM:28:ALA:HB3  | 2.61                     | 0.40              |
| 1:XA:1448:C:H42   | 1:XA:1455:G:H1    | 1.69                     | 0.40              |
| 3:XC:55:VAL:O     | 3:XC:55:VAL:HG12  | 2.20                     | 0.40              |
| 3:XC:70:VAL:CG1   | 3:XC:71:ALA:H     | 2.35                     | 0.40              |
| 3:XC:108:ASN:HB3  | 3:XC:111:LEU:CD1  | 2.52                     | 0.40              |
| 3:XC:120:VAL:O    | 3:XC:123:GLN:HB2  | 2.20                     | 0.40              |
| 3:XC:178:LEU:C    | 3:XC:180:ALA:H    | 2.29                     | 0.40              |
| 4:XD:178:VAL:O    | 4:XD:179:GLU:C    | 2.63                     | 0.40              |
| 4:XD:199:ASN:C    | 4:XD:201:GLN:N    | 2.79                     | 0.40              |
| 4:XD:199:ASN:OD1  | 4:XD:201:GLN:HB3  | 2.21                     | 0.40              |
| 8:XH:41:ARG:CG    | 8:XH:41:ARG:NH1   | 2.76                     | 0.40              |
| 8:XH:97:VAL:O     | 8:XH:100:ILE:HG13 | 2.21                     | 0.40              |
| 10:XJ:45:ARG:HB2  | 10:XJ:65:LEU:HB3  | 2.03                     | 0.40              |
| 10:XJ:65:LEU:HA   | 14:XM:55:GLY:O    | 2.21                     | 0.40              |
| 11:XK:83:ILE:HG12 | 11:XK:109:VAL:CG2 | 2.51                     | 0.40              |
| 12:XL:21:LYS:N    | 12:XL:21:LYS:CD   | 2.83                     | 0.40              |
| 12:XL:91:LYS:HE2  | 12:XL:91:LYS:HB2  | 1.76                     | 0.40              |
| 15:XO:70:LEU:HD23 | 15:XO:81:LEU:HD23 | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:XQ:83:ASP:O    | 17:XQ:87:LYS:HG2  | 2.22                     | 0.40              |
| 19:XS:29:ARG:HG2  | 19:XS:29:ARG:NH1  | 2.37                     | 0.40              |
| 20:XT:49:ALA:HA   | 20:XT:92:LEU:HD21 | 2.03                     | 0.40              |
| 22:XV:74:C:H2'    | 22:XV:75:C:H5'    | 2.03                     | 0.40              |
| 25:YA:1252:G:C2   | 25:YA:1253:A:C2   | 3.10                     | 0.40              |
| 25:YA:2150:U:H2'  | 25:YA:2151:G:C8   | 2.55                     | 0.40              |
| 25:YA:2212:A:N3   | 25:YA:2215:G:N1   | 2.69                     | 0.40              |
| 25:YA:2642:G:H5'' | 33:YN:78:TYR:CD2  | 2.57                     | 0.40              |
| 27:YD:107:ALA:HA  | 27:YD:108:PRO:HD2 | 2.01                     | 0.40              |
| 29:YF:118:ALA:C   | 29:YF:120:GLU:N   | 2.78                     | 0.40              |
| 29:YF:150:GLY:C   | 29:YF:152:GLU:H   | 2.29                     | 0.40              |
| 36:YQ:39:PRO:HA   | 36:YQ:97:VAL:O    | 2.21                     | 0.40              |
| 38:YS:62:LYS:CB   | 38:YS:97:ARG:HD3  | 2.46                     | 0.40              |
| 38:YS:83:LYS:HE3  | 38:YS:84:GLN:HG3  | 2.02                     | 0.40              |
| 40:YU:30:LYS:HA   | 40:YU:30:LYS:HD3  | 1.84                     | 0.40              |
| 40:YU:33:ARG:O    | 40:YU:37:GLU:HB2  | 2.21                     | 0.40              |
| 44:YY:95:LYS:HA   | 44:YY:101:LYS:CB  | 2.51                     | 0.40              |
| 44:YY:98:VAL:O    | 44:YY:99:CYS:HB3  | 2.21                     | 0.40              |
| 47:Y1:96:LYS:O    | 47:Y1:96:LYS:HG2  | 2.21                     | 0.40              |
| 50:Y4:42:PHE:CZ   | 50:Y4:43:TYR:HB3  | 2.57                     | 0.40              |
| 50:Y4:52:THR:O    | 50:Y4:53:GLU:CB   | 2.69                     | 0.40              |
| 54:Y8:39:LYS:HD2  | 54:Y8:39:LYS:O    | 2.22                     | 0.40              |
| 1:QA:186(A):C:H2' | 1:QA:186(B):C:C6  | 2.57                     | 0.40              |
| 1:QA:603:U:H3     | 1:QA:635:G:H1     | 1.69                     | 0.40              |
| 1:QA:1072:G:C5    | 1:QA:1073:U:C4    | 3.09                     | 0.40              |
| 1:QA:1485:U:H2'   | 1:QA:1486:G:C8    | 2.56                     | 0.40              |
| 2:QB:5:ILE:CG2    | 2:QB:224:GLN:HG2  | 2.51                     | 0.40              |
| 2:QB:132:LYS:HA   | 2:QB:135:GLN:CG   | 2.52                     | 0.40              |
| 3:QC:59:ARG:HH12  | 3:QC:97:LYS:CE    | 2.33                     | 0.40              |
| 4:QD:172:PRO:C    | 4:QD:174:LEU:H    | 2.29                     | 0.40              |
| 4:QD:206:PHE:CD2  | 4:QD:207:TYR:HD1  | 2.37                     | 0.40              |
| 6:QF:61:LEU:HB3   | 6:QF:63:TYR:CE2   | 2.53                     | 0.40              |
| 7:QG:62:PHE:C     | 7:QG:64:GLN:N     | 2.79                     | 0.40              |
| 7:QG:64:GLN:C     | 7:QG:66:VAL:N     | 2.77                     | 0.40              |
| 8:QH:36:LEU:O     | 8:QH:45:ILE:HD11  | 2.21                     | 0.40              |
| 8:QH:44:PHE:HA    | 8:QH:79:VAL:CG1   | 2.52                     | 0.40              |
| 8:QH:97:VAL:O     | 8:QH:100:ILE:HG13 | 2.21                     | 0.40              |
| 13:QM:54:VAL:O    | 13:QM:54:VAL:HG12 | 2.21                     | 0.40              |
| 16:QP:20:VAL:CG2  | 16:QP:32:TYR:CD2  | 3.04                     | 0.40              |
| 16:QP:22:THR:CA   | 16:QP:33:ILE:HG12 | 2.42                     | 0.40              |
| 17:QQ:8:GLY:HA3   | 17:QQ:21:VAL:HG12 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:QQ:60:ILE:O    | 17:QQ:60:ILE:HG23 | 2.21                     | 0.40              |
| 19:QS:10:PHE:CD2  | 19:QS:11:VAL:N    | 2.90                     | 0.40              |
| 20:QT:82:SER:O    | 20:QT:86:ARG:CB   | 2.70                     | 0.40              |
| 22:QV:74:C:H2'    | 22:QV:75:C:H5'    | 2.03                     | 0.40              |
| 25:RA:69:C:O2     | 25:RA:73:A:O2'    | 2.33                     | 0.40              |
| 25:RA:957:A:H5'   | 36:RQ:76:LYS:CD   | 2.43                     | 0.40              |
| 25:RA:990:A:H1'   | 25:RA:1156:A:N3   | 2.36                     | 0.40              |
| 25:RA:2093:G:H21  | 25:RA:2198:A:H62  | 1.70                     | 0.40              |
| 25:RA:2481:G:H4'  | 25:RA:2482:G:H5'  | 2.03                     | 0.40              |
| 26:RB:17:C:H2'    | 26:RB:18:G:O4'    | 2.22                     | 0.40              |
| 28:RE:92:THR:HB   | 28:RE:93:VAL:H    | 1.57                     | 0.40              |
| 29:RF:33:LEU:O    | 29:RF:37:VAL:HG23 | 2.21                     | 0.40              |
| 31:RH:20:ALA:HB3  | 31:RH:23:ARG:HG2  | 2.03                     | 0.40              |
| 31:RH:52:VAL:HG21 | 31:RH:68:THR:HG22 | 2.03                     | 0.40              |
| 31:RH:146:ALA:HB2 | 31:RH:164:TYR:OH  | 2.20                     | 0.40              |
| 33:RN:39:ARG:C    | 33:RN:41:ASP:H    | 2.28                     | 0.40              |
| 33:RN:75:TYR:O    | 33:RN:76:SER:O    | 2.40                     | 0.40              |
| 33:RN:89:LYS:O    | 33:RN:90:MET:C    | 2.65                     | 0.40              |
| 34:RO:67:LYS:O    | 34:RO:68:GLU:C    | 2.63                     | 0.40              |
| 35:RP:2:LYS:O     | 35:RP:5:ASP:CB    | 2.70                     | 0.40              |
| 36:RQ:51:ARG:O    | 36:RQ:52:VAL:C    | 2.62                     | 0.40              |
| 38:RS:83:LYS:CE   | 38:RS:109:GLY:HA2 | 2.47                     | 0.40              |
| 39:RT:20:PRO:HG2  | 39:RT:86:ILE:O    | 2.21                     | 0.40              |
| 39:RT:23:ARG:O    | 39:RT:49:VAL:HG11 | 2.21                     | 0.40              |
| 40:RU:62:ILE:HG23 | 40:RU:76:TYR:CE1  | 2.57                     | 0.40              |
| 44:RY:94:LYS:HE3  | 44:RY:101:LYS:HZ1 | 1.82                     | 0.40              |
| 45:RZ:119:GLU:CD  | 45:RZ:119:GLU:H   | 2.29                     | 0.40              |
| 47:R1:86:SER:O    | 47:R1:89:GLU:HB2  | 2.21                     | 0.40              |
| 52:R6:36:LEU:HD23 | 52:R6:36:LEU:N    | 2.37                     | 0.40              |
| 1:XA:110:C:H2'    | 1:XA:111:G:O4'    | 2.21                     | 0.40              |
| 1:XA:244:U:H4'    | 1:XA:245:C:O5'    | 2.20                     | 0.40              |
| 1:XA:349:A:O2'    | 1:XA:350:G:H5'    | 2.22                     | 0.40              |
| 1:XA:1127:G:H2'   | 1:XA:1128:C:C6    | 2.56                     | 0.40              |
| 1:XA:1347:G:OP2   | 9:XI:107:ARG:HG2  | 2.20                     | 0.40              |
| 2:XB:47:THR:O     | 2:XB:51:LEU:N     | 2.32                     | 0.40              |
| 5:XE:36:ASP:O     | 5:XE:37:ARG:HG2   | 2.22                     | 0.40              |
| 7:XG:50:ILE:HA    | 7:XG:54:THR:CG2   | 2.52                     | 0.40              |
| 8:XH:53:VAL:HG12  | 8:XH:54:ASP:OD2   | 2.20                     | 0.40              |
| 11:XK:20:TYR:O    | 11:XK:30:VAL:HA   | 2.21                     | 0.40              |
| 12:XL:45:PRO:C    | 12:XL:46:LYS:O    | 2.63                     | 0.40              |
| 13:XM:119:GLY:O   | 13:XM:120:LYS:O   | 2.38                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1045:A:O2'  | 25:YA:1046:A:OP2   | 2.30                     | 0.40              |
| 25:YA:1790:C:H2'  | 25:YA:1791:A:C5    | 2.57                     | 0.40              |
| 25:YA:2789:C:H1'  | 25:YA:2892:A:C2    | 2.48                     | 0.40              |
| 29:YF:160:ASN:O   | 29:YF:161:GLU:C    | 2.64                     | 0.40              |
| 30:YG:135:LEU:N   | 30:YG:135:LEU:CD1  | 2.83                     | 0.40              |
| 34:YO:7:TYR:CE1   | 34:YO:20:MET:HE3   | 2.53                     | 0.40              |
| 34:YO:47:ILE:HD12 | 34:YO:48:PRO:CD    | 2.44                     | 0.40              |
| 34:YO:67:LYS:O    | 34:YO:68:GLU:C     | 2.63                     | 0.40              |
| 35:YP:2:LYS:O     | 35:YP:5:ASP:CB     | 2.70                     | 0.40              |
| 37:YR:18:LEU:HD11 | 37:YR:22:ARG:NE    | 2.36                     | 0.40              |
| 38:YS:24:LEU:HD22 | 38:YS:24:LEU:N     | 2.37                     | 0.40              |
| 39:YT:23:ARG:O    | 39:YT:24:PRO:C     | 2.65                     | 0.40              |
| 39:YT:26:ASP:HB3  | 39:YT:92:GLY:H     | 1.87                     | 0.40              |
| 42:YW:51:LEU:CD2  | 42:YW:105:VAL:HG11 | 2.51                     | 0.40              |
| 42:YW:88:ARG:HA   | 42:YW:88:ARG:HD2   | 1.92                     | 0.40              |
| 44:YY:97:ARG:O    | 44:YY:97:ARG:CG    | 2.70                     | 0.40              |
| 48:Y2:37:PHE:O    | 48:Y2:40:SER:HB3   | 2.22                     | 0.40              |
| 50:Y4:61:ARG:C    | 50:Y4:63:TYR:N     | 2.73                     | 0.40              |

All (17) 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) |
|------------------|-------------------------|--------------------------|-------------------|
| 41:YV:50:PRO:C   | 51:Y5:60:VAL:O[4_445]   | 1.47                     | 0.73              |
| 41:YV:51:VAL:N   | 51:Y5:60:VAL:O[4_445]   | 1.50                     | 0.70              |
| 41:YV:51:VAL:N   | 51:Y5:60:VAL:C[4_445]   | 1.60                     | 0.60              |
| 41:YV:50:PRO:CG  | 51:Y5:60:VAL:CA[4_445]  | 1.78                     | 0.42              |
| 41:YV:50:PRO:CA  | 51:Y5:60:VAL:O[4_445]   | 1.83                     | 0.37              |
| 41:YV:50:PRO:N   | 51:Y5:60:VAL:O[4_445]   | 1.85                     | 0.35              |
| 41:YV:51:VAL:N   | 51:Y5:60:VAL:OXT[4_445] | 1.88                     | 0.32              |
| 41:YV:51:VAL:CA  | 51:Y5:60:VAL:OXT[4_445] | 1.89                     | 0.31              |
| 41:YV:53:GLU:OE1 | 51:Y5:57:VAL:CG2[4_445] | 1.94                     | 0.26              |
| 6:QF:15:ASP:OD2  | 4:XD:27:TYR:OH[4_555]   | 2.06                     | 0.14              |
| 41:YV:49:THR:CB  | 51:Y5:59:GLU:O[4_445]   | 2.07                     | 0.13              |
| 25:RA:1413:G:O2' | 30:RG:9:ARG:NH2[1_655]  | 2.08                     | 0.12              |
| 41:YV:50:PRO:CD  | 51:Y5:59:GLU:O[4_445]   | 2.08                     | 0.12              |
| 41:YV:51:VAL:CB  | 51:Y5:60:VAL:OXT[4_445] | 2.12                     | 0.08              |
| 41:YV:51:VAL:C   | 51:Y5:60:VAL:OXT[4_445] | 2.15                     | 0.05              |
| 25:YA:1473:G:O2' | 30:YG:21:ARG:NH1[1_655] | 2.16                     | 0.04              |
| 49:R3:2:PRO:CD   | 35:YP:122:PRO:CD[3_455] | 2.18                     | 0.02              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | QB    | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0           | 3  |
| 2   | XB    | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0           | 3  |
| 3   | QC    | 203/239 (85%) | 128 (63%) | 56 (28%) | 19 (9%)  | 0           | 6  |
| 3   | XC    | 203/239 (85%) | 129 (64%) | 55 (27%) | 19 (9%)  | 0           | 6  |
| 4   | QD    | 206/209 (99%) | 136 (66%) | 50 (24%) | 20 (10%) | 0           | 6  |
| 4   | XD    | 206/209 (99%) | 135 (66%) | 49 (24%) | 22 (11%) | 0           | 5  |
| 5   | QE    | 149/162 (92%) | 103 (69%) | 31 (21%) | 15 (10%) | 0           | 6  |
| 5   | XE    | 149/162 (92%) | 103 (69%) | 30 (20%) | 16 (11%) | 0           | 5  |
| 6   | QF    | 99/101 (98%)  | 66 (67%)  | 24 (24%) | 9 (9%)   | 0           | 7  |
| 6   | XF    | 99/101 (98%)  | 66 (67%)  | 24 (24%) | 9 (9%)   | 0           | 7  |
| 7   | QG    | 153/156 (98%) | 102 (67%) | 36 (24%) | 15 (10%) | 0           | 6  |
| 7   | XG    | 153/156 (98%) | 103 (67%) | 36 (24%) | 14 (9%)  | 0           | 6  |
| 8   | QH    | 136/138 (99%) | 92 (68%)  | 29 (21%) | 15 (11%) | 0           | 5  |
| 8   | XH    | 136/138 (99%) | 92 (68%)  | 29 (21%) | 15 (11%) | 0           | 5  |
| 9   | QI    | 125/128 (98%) | 77 (62%)  | 32 (26%) | 16 (13%) | 0           | 3  |
| 9   | XI    | 125/128 (98%) | 77 (62%)  | 32 (26%) | 16 (13%) | 0           | 3  |
| 10  | QJ    | 97/105 (92%)  | 68 (70%)  | 20 (21%) | 9 (9%)   | 0           | 6  |
| 10  | XJ    | 97/105 (92%)  | 68 (70%)  | 19 (20%) | 10 (10%) | 0           | 5  |
| 11  | QK    | 117/129 (91%) | 87 (74%)  | 22 (19%) | 8 (7%)   | 1           | 10 |
| 11  | XK    | 117/129 (91%) | 87 (74%)  | 21 (18%) | 9 (8%)   | 1           | 8  |
| 12  | QL    | 123/132 (93%) | 85 (69%)  | 24 (20%) | 14 (11%) | 0           | 5  |
| 12  | XL    | 123/132 (93%) | 85 (69%)  | 24 (20%) | 14 (11%) | 0           | 5  |
| 13  | QM    | 119/126 (94%) | 71 (60%)  | 28 (24%) | 20 (17%) | 0           | 2  |
| 13  | XM    | 119/126 (94%) | 71 (60%)  | 28 (24%) | 20 (17%) | 0           | 2  |
| 14  | QN    | 58/61 (95%)   | 31 (53%)  | 15 (26%) | 12 (21%) | 0           | 1  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 14  | XN    | 58/61 (95%)   | 32 (55%)  | 14 (24%) | 12 (21%) | 0           | 1  |
| 15  | QO    | 86/89 (97%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 10 |
| 15  | XO    | 86/89 (97%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 10 |
| 16  | QP    | 82/88 (93%)   | 48 (58%)  | 23 (28%) | 11 (13%) | 0           | 3  |
| 16  | XP    | 82/88 (93%)   | 48 (58%)  | 23 (28%) | 11 (13%) | 0           | 3  |
| 17  | QQ    | 98/105 (93%)  | 75 (76%)  | 15 (15%) | 8 (8%)   | 0           | 8  |
| 17  | XQ    | 98/105 (93%)  | 75 (76%)  | 15 (15%) | 8 (8%)   | 0           | 8  |
| 18  | QR    | 68/88 (77%)   | 45 (66%)  | 15 (22%) | 8 (12%)  | 0           | 4  |
| 18  | XR    | 68/88 (77%)   | 45 (66%)  | 15 (22%) | 8 (12%)  | 0           | 4  |
| 19  | QS    | 82/93 (88%)   | 47 (57%)  | 17 (21%) | 18 (22%) | 0           | 1  |
| 19  | XS    | 82/93 (88%)   | 46 (56%)  | 18 (22%) | 18 (22%) | 0           | 1  |
| 20  | QT    | 97/106 (92%)  | 63 (65%)  | 15 (16%) | 19 (20%) | 0           | 1  |
| 20  | XT    | 97/106 (92%)  | 63 (65%)  | 15 (16%) | 19 (20%) | 0           | 1  |
| 21  | QU    | 23/27 (85%)   | 15 (65%)  | 4 (17%)  | 4 (17%)  | 0           | 2  |
| 21  | XU    | 23/27 (85%)   | 16 (70%)  | 3 (13%)  | 4 (17%)  | 0           | 2  |
| 27  | RD    | 270/276 (98%) | 203 (75%) | 48 (18%) | 19 (7%)  | 1           | 10 |
| 27  | YD    | 270/276 (98%) | 204 (76%) | 47 (17%) | 19 (7%)  | 1           | 10 |
| 28  | RE    | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0           | 1  |
| 28  | YE    | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0           | 1  |
| 29  | RF    | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 0           | 6  |
| 29  | YF    | 200/210 (95%) | 143 (72%) | 37 (18%) | 20 (10%) | 0           | 6  |
| 30  | RG    | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 0           | 4  |
| 30  | YG    | 179/182 (98%) | 120 (67%) | 38 (21%) | 21 (12%) | 0           | 4  |
| 31  | RH    | 168/180 (93%) | 94 (56%)  | 36 (21%) | 38 (23%) | 0           | 1  |
| 31  | YH    | 168/180 (93%) | 94 (56%)  | 36 (21%) | 38 (23%) | 0           | 1  |
| 32  | RI    | 144/148 (97%) | 102 (71%) | 29 (20%) | 13 (9%)  | 0           | 7  |
| 32  | YI    | 144/148 (97%) | 101 (70%) | 26 (18%) | 17 (12%) | 0           | 4  |
| 33  | RN    | 136/140 (97%) | 84 (62%)  | 30 (22%) | 22 (16%) | 0           | 2  |
| 33  | YN    | 136/140 (97%) | 84 (62%)  | 30 (22%) | 22 (16%) | 0           | 2  |
| 34  | RO    | 120/122 (98%) | 90 (75%)  | 21 (18%) | 9 (8%)   | 1           | 9  |
| 34  | YO    | 120/122 (98%) | 90 (75%)  | 21 (18%) | 9 (8%)   | 1           | 9  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35  | RP    | 148/150 (99%) | 97 (66%)  | 19 (13%) | 32 (22%) | 0           | 1   |
| 35  | YP    | 148/150 (99%) | 97 (66%)  | 19 (13%) | 32 (22%) | 0           | 1   |
| 36  | RQ    | 139/141 (99%) | 95 (68%)  | 30 (22%) | 14 (10%) | 0           | 6   |
| 36  | YQ    | 139/141 (99%) | 97 (70%)  | 28 (20%) | 14 (10%) | 0           | 6   |
| 37  | RR    | 116/118 (98%) | 83 (72%)  | 19 (16%) | 14 (12%) | 0           | 4   |
| 37  | YR    | 116/118 (98%) | 82 (71%)  | 20 (17%) | 14 (12%) | 0           | 4   |
| 38  | RS    | 109/112 (97%) | 62 (57%)  | 28 (26%) | 19 (17%) | 0           | 2   |
| 38  | YS    | 109/112 (97%) | 63 (58%)  | 27 (25%) | 19 (17%) | 0           | 2   |
| 39  | RT    | 135/146 (92%) | 83 (62%)  | 32 (24%) | 20 (15%) | 0           | 2   |
| 39  | YT    | 135/146 (92%) | 83 (62%)  | 32 (24%) | 20 (15%) | 0           | 2   |
| 40  | RU    | 115/118 (98%) | 86 (75%)  | 20 (17%) | 9 (8%)   | 1           | 8   |
| 40  | YU    | 115/118 (98%) | 86 (75%)  | 20 (17%) | 9 (8%)   | 1           | 8   |
| 41  | RV    | 99/101 (98%)  | 73 (74%)  | 16 (16%) | 10 (10%) | 0           | 6   |
| 41  | YV    | 99/101 (98%)  | 73 (74%)  | 16 (16%) | 10 (10%) | 0           | 6   |
| 42  | RW    | 111/113 (98%) | 75 (68%)  | 22 (20%) | 14 (13%) | 0           | 4   |
| 42  | YW    | 111/113 (98%) | 75 (68%)  | 22 (20%) | 14 (13%) | 0           | 4   |
| 43  | RX    | 90/96 (94%)   | 77 (86%)  | 8 (9%)   | 5 (6%)   | 1           | 13  |
| 43  | YX    | 90/96 (94%)   | 77 (86%)  | 8 (9%)   | 5 (6%)   | 1           | 13  |
| 44  | RY    | 100/110 (91%) | 58 (58%)  | 16 (16%) | 26 (26%) | 0           | 0   |
| 44  | YY    | 100/110 (91%) | 57 (57%)  | 17 (17%) | 26 (26%) | 0           | 0   |
| 45  | RZ    | 181/206 (88%) | 126 (70%) | 40 (22%) | 15 (8%)  | 0           | 7   |
| 45  | YZ    | 181/206 (88%) | 125 (69%) | 38 (21%) | 18 (10%) | 0           | 6   |
| 46  | R0    | 80/85 (94%)   | 68 (85%)  | 9 (11%)  | 3 (4%)   | 2           | 20  |
| 46  | Y0    | 80/85 (94%)   | 71 (89%)  | 9 (11%)  | 0        | 100         | 100 |
| 47  | R1    | 95/98 (97%)   | 64 (67%)  | 20 (21%) | 11 (12%) | 0           | 5   |
| 47  | Y1    | 95/98 (97%)   | 64 (67%)  | 20 (21%) | 11 (12%) | 0           | 5   |
| 48  | R2    | 67/72 (93%)   | 46 (69%)  | 12 (18%) | 9 (13%)  | 0           | 3   |
| 48  | Y2    | 67/72 (93%)   | 47 (70%)  | 11 (16%) | 9 (13%)  | 0           | 3   |
| 49  | R3    | 57/60 (95%)   | 45 (79%)  | 9 (16%)  | 3 (5%)   | 1           | 14  |
| 49  | Y3    | 57/60 (95%)   | 45 (79%)  | 9 (16%)  | 3 (5%)   | 1           | 14  |
| 50  | R4    | 69/71 (97%)   | 23 (33%)  | 20 (29%) | 26 (38%) | 0           | 0   |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-------------------|------------|------------|------------|-------------|-----|
| 50  | Y4    | 69/71 (97%)       | 23 (33%)   | 20 (29%)   | 26 (38%)   | 0           | 0   |
| 51  | R5    | 57/60 (95%)       | 33 (58%)   | 9 (16%)    | 15 (26%)   | 0           | 0   |
| 51  | Y5    | 57/60 (95%)       | 33 (58%)   | 9 (16%)    | 15 (26%)   | 0           | 0   |
| 52  | R6    | 47/54 (87%)       | 15 (32%)   | 18 (38%)   | 14 (30%)   | 0           | 0   |
| 52  | Y6    | 47/54 (87%)       | 15 (32%)   | 18 (38%)   | 14 (30%)   | 0           | 0   |
| 53  | R7    | 47/49 (96%)       | 37 (79%)   | 7 (15%)    | 3 (6%)     | 1           | 11  |
| 53  | Y7    | 47/49 (96%)       | 37 (79%)   | 7 (15%)    | 3 (6%)     | 1           | 11  |
| 54  | R8    | 62/65 (95%)       | 36 (58%)   | 15 (24%)   | 11 (18%)   | 0           | 1   |
| 54  | Y8    | 62/65 (95%)       | 36 (58%)   | 15 (24%)   | 11 (18%)   | 0           | 1   |
| 55  | R9    | 35/37 (95%)       | 31 (89%)   | 4 (11%)    | 0          | 100         | 100 |
| 55  | Y9    | 35/37 (95%)       | 31 (89%)   | 4 (11%)    | 0          | 100         | 100 |
| All | All   | 11470/12128 (95%) | 7650 (67%) | 2346 (20%) | 1474 (13%) | 0           | 3   |

All (1474) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 6   | THR  |
| 2   | QB    | 15  | VAL  |
| 2   | QB    | 26  | PRO  |
| 2   | QB    | 84  | GLU  |
| 2   | QB    | 88  | ALA  |
| 2   | QB    | 126 | GLU  |
| 2   | QB    | 230 | VAL  |
| 2   | QB    | 233 | SER  |
| 3   | QC    | 4   | LYS  |
| 3   | QC    | 12  | LEU  |
| 3   | QC    | 14  | ILE  |
| 3   | QC    | 29  | TYR  |
| 3   | QC    | 61  | ALA  |
| 3   | QC    | 189 | ALA  |
| 3   | QC    | 190 | ARG  |
| 4   | QD    | 28  | SER  |
| 4   | QD    | 29  | PRO  |
| 4   | QD    | 51  | PRO  |
| 4   | QD    | 89  | THR  |
| 4   | QD    | 129 | ASN  |
| 4   | QD    | 154 | ASN  |
| 4   | QD    | 155 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | QD    | 178 | VAL  |
| 5   | QE    | 146 | ALA  |
| 7   | QG    | 5   | ARG  |
| 7   | QG    | 7   | ALA  |
| 8   | QH    | 50  | ARG  |
| 8   | QH    | 129 | VAL  |
| 9   | QI    | 23  | ASN  |
| 9   | QI    | 56  | LEU  |
| 9   | QI    | 95  | LYS  |
| 9   | QI    | 111 | ARG  |
| 9   | QI    | 117 | HIS  |
| 10  | QJ    | 30  | SER  |
| 10  | QJ    | 33  | GLN  |
| 11  | QK    | 91  | ARG  |
| 12  | QL    | 18  | VAL  |
| 12  | QL    | 27  | LEU  |
| 12  | QL    | 48  | PRO  |
| 12  | QL    | 62  | SER  |
| 12  | QL    | 121 | GLY  |
| 13  | QM    | 67  | GLU  |
| 13  | QM    | 70  | LEU  |
| 13  | QM    | 83  | ASP  |
| 13  | QM    | 106 | ASN  |
| 13  | QM    | 108 | ARG  |
| 13  | QM    | 118 | ALA  |
| 14  | QN    | 3   | ARG  |
| 14  | QN    | 16  | PHE  |
| 14  | QN    | 23  | ARG  |
| 14  | QN    | 24  | CYS  |
| 14  | QN    | 44  | LEU  |
| 15  | QO    | 88  | ARG  |
| 16  | QP    | 44  | THR  |
| 16  | QP    | 67  | THR  |
| 17  | QQ    | 34  | LYS  |
| 17  | QQ    | 49  | GLU  |
| 18  | QR    | 22  | VAL  |
| 19  | QS    | 3   | ARG  |
| 19  | QS    | 12  | ASP  |
| 19  | QS    | 14  | HIS  |
| 19  | QS    | 25  | LYS  |
| 19  | QS    | 26  | GLY  |
| 19  | QS    | 31  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | QS    | 41  | VAL  |
| 19  | QS    | 70  | LYS  |
| 19  | QS    | 78  | ARG  |
| 19  | QS    | 79  | THR  |
| 20  | QT    | 48  | LYS  |
| 20  | QT    | 49  | ALA  |
| 20  | QT    | 74  | LYS  |
| 20  | QT    | 95  | ALA  |
| 20  | QT    | 96  | GLY  |
| 20  | QT    | 100 | ILE  |
| 21  | QU    | 7   | ARG  |
| 21  | QU    | 9   | ARG  |
| 21  | QU    | 22  | ARG  |
| 27  | RD    | 26  | LYS  |
| 27  | RD    | 28  | GLU  |
| 27  | RD    | 123 | ALA  |
| 27  | RD    | 231 | HIS  |
| 28  | RE    | 4   | ILE  |
| 28  | RE    | 7   | VAL  |
| 28  | RE    | 9   | VAL  |
| 28  | RE    | 22  | PRO  |
| 28  | RE    | 54  | GLN  |
| 28  | RE    | 57  | LYS  |
| 28  | RE    | 60  | ASN  |
| 28  | RE    | 63  | LEU  |
| 28  | RE    | 64  | LYS  |
| 28  | RE    | 68  | ALA  |
| 28  | RE    | 70  | ALA  |
| 28  | RE    | 73  | GLU  |
| 28  | RE    | 90  | THR  |
| 28  | RE    | 92  | THR  |
| 28  | RE    | 93  | VAL  |
| 28  | RE    | 169 | ASN  |
| 28  | RE    | 187 | ALA  |
| 28  | RE    | 189 | PRO  |
| 29  | RF    | 25  | PRO  |
| 29  | RF    | 66  | PRO  |
| 29  | RF    | 68  | LYS  |
| 29  | RF    | 73  | ALA  |
| 29  | RF    | 89  | VAL  |
| 29  | RF    | 128 | ALA  |
| 29  | RF    | 176 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | RG    | 4   | ASP  |
| 30  | RG    | 14  | GLU  |
| 30  | RG    | 79  | ASN  |
| 30  | RG    | 86  | MET  |
| 31  | RH    | 10  | PRO  |
| 31  | RH    | 12  | PRO  |
| 31  | RH    | 83  | TYR  |
| 31  | RH    | 85  | LYS  |
| 31  | RH    | 86  | GLU  |
| 31  | RH    | 87  | LEU  |
| 31  | RH    | 90  | LYS  |
| 31  | RH    | 92  | ILE  |
| 31  | RH    | 126 | PRO  |
| 31  | RH    | 127 | GLU  |
| 31  | RH    | 128 | PRO  |
| 31  | RH    | 137 | ASP  |
| 31  | RH    | 138 | LYS  |
| 31  | RH    | 153 | LYS  |
| 31  | RH    | 154 | PRO  |
| 31  | RH    | 155 | SER  |
| 31  | RH    | 169 | VAL  |
| 32  | RI    | 10  | GLU  |
| 32  | RI    | 115 | ALA  |
| 33  | RN    | 6   | PRO  |
| 33  | RN    | 9   | VAL  |
| 33  | RN    | 22  | THR  |
| 33  | RN    | 36  | GLY  |
| 33  | RN    | 58  | ASP  |
| 33  | RN    | 95  | PRO  |
| 33  | RN    | 97  | ARG  |
| 33  | RN    | 119 | ARG  |
| 33  | RN    | 131 | GLN  |
| 33  | RN    | 133 | GLN  |
| 33  | RN    | 134 | ARG  |
| 34  | RO    | 49  | ARG  |
| 35  | RP    | 5   | ASP  |
| 35  | RP    | 10  | PRO  |
| 35  | RP    | 15  | ARG  |
| 35  | RP    | 19  | VAL  |
| 35  | RP    | 21  | ARG  |
| 35  | RP    | 25  | SER  |
| 35  | RP    | 27  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | RP    | 36  | LYS  |
| 35  | RP    | 38  | GLN  |
| 35  | RP    | 42  | SER  |
| 35  | RP    | 65  | ARG  |
| 35  | RP    | 95  | VAL  |
| 35  | RP    | 106 | LEU  |
| 35  | RP    | 107 | LYS  |
| 35  | RP    | 141 | ALA  |
| 35  | RP    | 148 | LEU  |
| 36  | RQ    | 6   | ARG  |
| 36  | RQ    | 18  | LYS  |
| 36  | RQ    | 22  | LYS  |
| 36  | RQ    | 27  | VAL  |
| 36  | RQ    | 81  | VAL  |
| 36  | RQ    | 90  | VAL  |
| 36  | RQ    | 134 | ARG  |
| 37  | RR    | 2   | ARG  |
| 37  | RR    | 3   | HIS  |
| 37  | RR    | 4   | LEU  |
| 37  | RR    | 14  | SER  |
| 37  | RR    | 58  | GLY  |
| 37  | RR    | 86  | ARG  |
| 37  | RR    | 117 | VAL  |
| 38  | RS    | 4   | LEU  |
| 38  | RS    | 12  | PHE  |
| 38  | RS    | 14  | VAL  |
| 38  | RS    | 23  | ARG  |
| 38  | RS    | 56  | LEU  |
| 38  | RS    | 57  | LYS  |
| 38  | RS    | 88  | ASP  |
| 38  | RS    | 89  | ARG  |
| 38  | RS    | 90  | GLY  |
| 38  | RS    | 107 | GLU  |
| 39  | RT    | 2   | ASN  |
| 39  | RT    | 3   | ARG  |
| 39  | RT    | 39  | ARG  |
| 39  | RT    | 55  | ASN  |
| 39  | RT    | 58  | ASN  |
| 39  | RT    | 90  | GLN  |
| 39  | RT    | 94  | ALA  |
| 39  | RT    | 97  | ALA  |
| 39  | RT    | 106 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | RT    | 107 | ASP  |
| 41  | RV    | 28  | GLU  |
| 41  | RV    | 31  | ALA  |
| 41  | RV    | 45  | THR  |
| 41  | RV    | 48  | GLY  |
| 41  | RV    | 49  | THR  |
| 41  | RV    | 50  | PRO  |
| 41  | RV    | 53  | GLU  |
| 41  | RV    | 79  | VAL  |
| 42  | RW    | 59  | VAL  |
| 42  | RW    | 67  | ASP  |
| 42  | RW    | 75  | TYR  |
| 42  | RW    | 111 | HIS  |
| 43  | RX    | 36  | LYS  |
| 44  | RY    | 3   | VAL  |
| 44  | RY    | 4   | LYS  |
| 44  | RY    | 23  | ARG  |
| 44  | RY    | 48  | ALA  |
| 44  | RY    | 49  | VAL  |
| 44  | RY    | 50  | ARG  |
| 44  | RY    | 53  | PRO  |
| 44  | RY    | 58  | GLY  |
| 44  | RY    | 63  | LYS  |
| 44  | RY    | 77  | PRO  |
| 44  | RY    | 78  | ALA  |
| 44  | RY    | 96  | ILE  |
| 45  | RZ    | 6   | LYS  |
| 45  | RZ    | 111 | VAL  |
| 47  | R1    | 30  | VAL  |
| 47  | R1    | 54  | ALA  |
| 47  | R1    | 81  | LYS  |
| 47  | R1    | 82  | LEU  |
| 47  | R1    | 95  | LEU  |
| 48  | R2    | 16  | LEU  |
| 48  | R2    | 43  | GLN  |
| 48  | R2    | 47  | ASN  |
| 48  | R2    | 48  | HIS  |
| 48  | R2    | 71  | ASN  |
| 49  | R3    | 3   | ARG  |
| 50  | R4    | 5   | ILE  |
| 50  | R4    | 14  | ILE  |
| 50  | R4    | 16  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | R4    | 22  | ILE  |
| 50  | R4    | 23  | GLU  |
| 50  | R4    | 36  | CYS  |
| 50  | R4    | 37  | SER  |
| 50  | R4    | 40  | HIS  |
| 50  | R4    | 42  | PHE  |
| 50  | R4    | 43  | TYR  |
| 50  | R4    | 49  | PHE  |
| 50  | R4    | 50  | VAL  |
| 50  | R4    | 51  | ASP  |
| 50  | R4    | 53  | GLU  |
| 50  | R4    | 62  | ARG  |
| 50  | R4    | 66  | SER  |
| 50  | R4    | 68  | ARG  |
| 51  | R5    | 3   | LYS  |
| 51  | R5    | 4   | HIS  |
| 51  | R5    | 35  | GLU  |
| 51  | R5    | 51  | TYR  |
| 51  | R5    | 53  | ALA  |
| 52  | R6    | 7   | ILE  |
| 52  | R6    | 14  | THR  |
| 52  | R6    | 15  | GLU  |
| 52  | R6    | 19  | ARG  |
| 52  | R6    | 21  | TYR  |
| 52  | R6    | 33  | LYS  |
| 52  | R6    | 45  | LYS  |
| 52  | R6    | 48  | VAL  |
| 54  | R8    | 29  | LYS  |
| 54  | R8    | 31  | HIS  |
| 54  | R8    | 34  | TRP  |
| 54  | R8    | 52  | LYS  |
| 54  | R8    | 62  | LEU  |
| 2   | XB    | 6   | THR  |
| 2   | XB    | 15  | VAL  |
| 2   | XB    | 26  | PRO  |
| 2   | XB    | 84  | GLU  |
| 2   | XB    | 88  | ALA  |
| 2   | XB    | 126 | GLU  |
| 2   | XB    | 230 | VAL  |
| 2   | XB    | 233 | SER  |
| 3   | XC    | 4   | LYS  |
| 3   | XC    | 12  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | XC    | 14  | ILE  |
| 3   | XC    | 29  | TYR  |
| 3   | XC    | 61  | ALA  |
| 3   | XC    | 189 | ALA  |
| 3   | XC    | 190 | ARG  |
| 4   | XD    | 28  | SER  |
| 4   | XD    | 30  | LYS  |
| 4   | XD    | 51  | PRO  |
| 4   | XD    | 89  | THR  |
| 4   | XD    | 129 | ASN  |
| 4   | XD    | 154 | ASN  |
| 4   | XD    | 155 | LEU  |
| 4   | XD    | 178 | VAL  |
| 5   | XE    | 146 | ALA  |
| 7   | XG    | 5   | ARG  |
| 7   | XG    | 7   | ALA  |
| 8   | XH    | 50  | ARG  |
| 8   | XH    | 129 | VAL  |
| 9   | XI    | 23  | ASN  |
| 9   | XI    | 56  | LEU  |
| 9   | XI    | 95  | LYS  |
| 9   | XI    | 111 | ARG  |
| 9   | XI    | 117 | HIS  |
| 10  | XJ    | 30  | SER  |
| 10  | XJ    | 33  | GLN  |
| 11  | XK    | 91  | ARG  |
| 12  | XL    | 18  | VAL  |
| 12  | XL    | 27  | LEU  |
| 12  | XL    | 48  | PRO  |
| 12  | XL    | 62  | SER  |
| 12  | XL    | 121 | GLY  |
| 13  | XM    | 67  | GLU  |
| 13  | XM    | 70  | LEU  |
| 13  | XM    | 83  | ASP  |
| 13  | XM    | 106 | ASN  |
| 13  | XM    | 108 | ARG  |
| 14  | XN    | 3   | ARG  |
| 14  | XN    | 16  | PHE  |
| 14  | XN    | 23  | ARG  |
| 14  | XN    | 43  | CYS  |
| 14  | XN    | 44  | LEU  |
| 15  | XO    | 88  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | XP    | 44  | THR  |
| 16  | XP    | 67  | THR  |
| 17  | XQ    | 34  | LYS  |
| 17  | XQ    | 49  | GLU  |
| 18  | XR    | 22  | VAL  |
| 19  | XS    | 3   | ARG  |
| 19  | XS    | 12  | ASP  |
| 19  | XS    | 14  | HIS  |
| 19  | XS    | 25  | LYS  |
| 19  | XS    | 26  | GLY  |
| 19  | XS    | 31  | ILE  |
| 19  | XS    | 41  | VAL  |
| 19  | XS    | 70  | LYS  |
| 19  | XS    | 78  | ARG  |
| 19  | XS    | 79  | THR  |
| 20  | XT    | 48  | LYS  |
| 20  | XT    | 49  | ALA  |
| 20  | XT    | 74  | LYS  |
| 20  | XT    | 95  | ALA  |
| 20  | XT    | 96  | GLY  |
| 20  | XT    | 100 | ILE  |
| 21  | XU    | 7   | ARG  |
| 21  | XU    | 9   | ARG  |
| 21  | XU    | 22  | ARG  |
| 27  | YD    | 26  | LYS  |
| 27  | YD    | 28  | GLU  |
| 27  | YD    | 123 | ALA  |
| 27  | YD    | 231 | HIS  |
| 28  | YE    | 4   | ILE  |
| 28  | YE    | 7   | VAL  |
| 28  | YE    | 9   | VAL  |
| 28  | YE    | 22  | PRO  |
| 28  | YE    | 54  | GLN  |
| 28  | YE    | 57  | LYS  |
| 28  | YE    | 60  | ASN  |
| 28  | YE    | 63  | LEU  |
| 28  | YE    | 64  | LYS  |
| 28  | YE    | 68  | ALA  |
| 28  | YE    | 70  | ALA  |
| 28  | YE    | 73  | GLU  |
| 28  | YE    | 90  | THR  |
| 28  | YE    | 92  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | YE    | 93  | VAL  |
| 28  | YE    | 169 | ASN  |
| 28  | YE    | 187 | ALA  |
| 28  | YE    | 189 | PRO  |
| 29  | YF    | 25  | PRO  |
| 29  | YF    | 66  | PRO  |
| 29  | YF    | 68  | LYS  |
| 29  | YF    | 73  | ALA  |
| 29  | YF    | 89  | VAL  |
| 29  | YF    | 128 | ALA  |
| 29  | YF    | 176 | LEU  |
| 30  | YG    | 4   | ASP  |
| 30  | YG    | 14  | GLU  |
| 30  | YG    | 79  | ASN  |
| 30  | YG    | 86  | MET  |
| 31  | YH    | 10  | PRO  |
| 31  | YH    | 12  | PRO  |
| 31  | YH    | 83  | TYR  |
| 31  | YH    | 85  | LYS  |
| 31  | YH    | 86  | GLU  |
| 31  | YH    | 87  | LEU  |
| 31  | YH    | 90  | LYS  |
| 31  | YH    | 92  | ILE  |
| 31  | YH    | 126 | PRO  |
| 31  | YH    | 127 | GLU  |
| 31  | YH    | 128 | PRO  |
| 31  | YH    | 137 | ASP  |
| 31  | YH    | 138 | LYS  |
| 31  | YH    | 153 | LYS  |
| 31  | YH    | 154 | PRO  |
| 31  | YH    | 155 | SER  |
| 31  | YH    | 169 | VAL  |
| 32  | YI    | 10  | GLU  |
| 32  | YI    | 133 | HIS  |
| 32  | YI    | 145 | VAL  |
| 33  | YN    | 6   | PRO  |
| 33  | YN    | 9   | VAL  |
| 33  | YN    | 22  | THR  |
| 33  | YN    | 36  | GLY  |
| 33  | YN    | 58  | ASP  |
| 33  | YN    | 95  | PRO  |
| 33  | YN    | 97  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | YN    | 119 | ARG  |
| 33  | YN    | 131 | GLN  |
| 33  | YN    | 133 | GLN  |
| 33  | YN    | 134 | ARG  |
| 34  | YO    | 49  | ARG  |
| 35  | YP    | 5   | ASP  |
| 35  | YP    | 10  | PRO  |
| 35  | YP    | 15  | ARG  |
| 35  | YP    | 19  | VAL  |
| 35  | YP    | 21  | ARG  |
| 35  | YP    | 25  | SER  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 36  | LYS  |
| 35  | YP    | 38  | GLN  |
| 35  | YP    | 42  | SER  |
| 35  | YP    | 65  | ARG  |
| 35  | YP    | 95  | VAL  |
| 35  | YP    | 106 | LEU  |
| 35  | YP    | 107 | LYS  |
| 35  | YP    | 141 | ALA  |
| 35  | YP    | 148 | LEU  |
| 36  | YQ    | 6   | ARG  |
| 36  | YQ    | 18  | LYS  |
| 36  | YQ    | 22  | LYS  |
| 36  | YQ    | 27  | VAL  |
| 36  | YQ    | 81  | VAL  |
| 36  | YQ    | 90  | VAL  |
| 36  | YQ    | 134 | ARG  |
| 37  | YR    | 2   | ARG  |
| 37  | YR    | 3   | HIS  |
| 37  | YR    | 4   | LEU  |
| 37  | YR    | 14  | SER  |
| 37  | YR    | 58  | GLY  |
| 37  | YR    | 86  | ARG  |
| 37  | YR    | 117 | VAL  |
| 38  | YS    | 4   | LEU  |
| 38  | YS    | 12  | PHE  |
| 38  | YS    | 14  | VAL  |
| 38  | YS    | 23  | ARG  |
| 38  | YS    | 56  | LEU  |
| 38  | YS    | 57  | LYS  |
| 38  | YS    | 88  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | YS    | 89  | ARG  |
| 38  | YS    | 90  | GLY  |
| 38  | YS    | 107 | GLU  |
| 39  | YT    | 2   | ASN  |
| 39  | YT    | 3   | ARG  |
| 39  | YT    | 39  | ARG  |
| 39  | YT    | 55  | ASN  |
| 39  | YT    | 58  | ASN  |
| 39  | YT    | 90  | GLN  |
| 39  | YT    | 94  | ALA  |
| 39  | YT    | 97  | ALA  |
| 39  | YT    | 106 | SER  |
| 39  | YT    | 107 | ASP  |
| 41  | YV    | 28  | GLU  |
| 41  | YV    | 31  | ALA  |
| 41  | YV    | 45  | THR  |
| 41  | YV    | 48  | GLY  |
| 41  | YV    | 49  | THR  |
| 41  | YV    | 50  | PRO  |
| 41  | YV    | 53  | GLU  |
| 41  | YV    | 79  | VAL  |
| 42  | YW    | 59  | VAL  |
| 42  | YW    | 67  | ASP  |
| 42  | YW    | 75  | TYR  |
| 42  | YW    | 111 | HIS  |
| 43  | YX    | 36  | LYS  |
| 44  | YY    | 3   | VAL  |
| 44  | YY    | 23  | ARG  |
| 44  | YY    | 48  | ALA  |
| 44  | YY    | 49  | VAL  |
| 44  | YY    | 50  | ARG  |
| 44  | YY    | 58  | GLY  |
| 44  | YY    | 63  | LYS  |
| 44  | YY    | 77  | PRO  |
| 44  | YY    | 78  | ALA  |
| 44  | YY    | 96  | ILE  |
| 45  | YZ    | 146 | ILE  |
| 45  | YZ    | 152 | ALA  |
| 45  | YZ    | 159 | PRO  |
| 45  | YZ    | 166 | SER  |
| 47  | Y1    | 30  | VAL  |
| 47  | Y1    | 54  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | Y1    | 81  | LYS  |
| 47  | Y1    | 82  | LEU  |
| 47  | Y1    | 95  | LEU  |
| 48  | Y2    | 16  | LEU  |
| 48  | Y2    | 43  | GLN  |
| 48  | Y2    | 47  | ASN  |
| 48  | Y2    | 48  | HIS  |
| 48  | Y2    | 71  | ASN  |
| 49  | Y3    | 3   | ARG  |
| 50  | Y4    | 5   | ILE  |
| 50  | Y4    | 14  | ILE  |
| 50  | Y4    | 16  | CYS  |
| 50  | Y4    | 22  | ILE  |
| 50  | Y4    | 23  | GLU  |
| 50  | Y4    | 36  | CYS  |
| 50  | Y4    | 37  | SER  |
| 50  | Y4    | 40  | HIS  |
| 50  | Y4    | 42  | PHE  |
| 50  | Y4    | 43  | TYR  |
| 50  | Y4    | 49  | PHE  |
| 50  | Y4    | 50  | VAL  |
| 50  | Y4    | 51  | ASP  |
| 50  | Y4    | 53  | GLU  |
| 50  | Y4    | 62  | ARG  |
| 50  | Y4    | 66  | SER  |
| 50  | Y4    | 68  | ARG  |
| 51  | Y5    | 3   | LYS  |
| 51  | Y5    | 4   | HIS  |
| 51  | Y5    | 35  | GLU  |
| 51  | Y5    | 51  | TYR  |
| 51  | Y5    | 53  | ALA  |
| 52  | Y6    | 7   | ILE  |
| 52  | Y6    | 14  | THR  |
| 52  | Y6    | 15  | GLU  |
| 52  | Y6    | 19  | ARG  |
| 52  | Y6    | 21  | TYR  |
| 52  | Y6    | 33  | LYS  |
| 52  | Y6    | 45  | LYS  |
| 52  | Y6    | 48  | VAL  |
| 54  | Y8    | 29  | LYS  |
| 54  | Y8    | 31  | HIS  |
| 54  | Y8    | 34  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | Y8    | 52  | LYS  |
| 54  | Y8    | 62  | LEU  |
| 2   | QB    | 18  | GLY  |
| 2   | QB    | 65  | GLY  |
| 2   | QB    | 208 | ILE  |
| 2   | QB    | 216 | SER  |
| 2   | QB    | 237 | ALA  |
| 3   | QC    | 60  | ALA  |
| 3   | QC    | 79  | ARG  |
| 3   | QC    | 129 | ALA  |
| 3   | QC    | 145 | GLY  |
| 4   | QD    | 7   | PRO  |
| 4   | QD    | 20  | TYR  |
| 4   | QD    | 164 | ALA  |
| 4   | QD    | 170 | VAL  |
| 4   | QD    | 179 | GLU  |
| 4   | QD    | 181 | MET  |
| 4   | QD    | 200 | GLU  |
| 5   | QE    | 21  | ALA  |
| 5   | QE    | 63  | ARG  |
| 5   | QE    | 108 | ALA  |
| 6   | QF    | 70  | ASP  |
| 7   | QG    | 4   | ARG  |
| 7   | QG    | 63  | LYS  |
| 7   | QG    | 141 | VAL  |
| 8   | QH    | 68  | ARG  |
| 8   | QH    | 69  | ARG  |
| 8   | QH    | 76  | PRO  |
| 8   | QH    | 122 | ARG  |
| 8   | QH    | 128 | GLY  |
| 9   | QI    | 31  | GLN  |
| 9   | QI    | 41  | VAL  |
| 9   | QI    | 100 | GLY  |
| 9   | QI    | 109 | VAL  |
| 10  | QJ    | 36  | GLY  |
| 10  | QJ    | 68  | HIS  |
| 11  | QK    | 103 | LEU  |
| 11  | QK    | 107 | SER  |
| 11  | QK    | 124 | LYS  |
| 11  | QK    | 125 | PHE  |
| 11  | QK    | 126 | ARG  |
| 12  | QL    | 65  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | QL    | 110 | VAL  |
| 12  | QL    | 115 | LYS  |
| 12  | QL    | 116 | SER  |
| 12  | QL    | 128 | ALA  |
| 13  | QM    | 49  | THR  |
| 13  | QM    | 68  | GLY  |
| 13  | QM    | 120 | LYS  |
| 14  | QN    | 14  | PRO  |
| 14  | QN    | 15  | LYS  |
| 14  | QN    | 27  | CYS  |
| 15  | QO    | 77  | ARG  |
| 16  | QP    | 49  | LEU  |
| 17  | QQ    | 14  | LYS  |
| 17  | QQ    | 33  | GLY  |
| 17  | QQ    | 78  | GLU  |
| 17  | QQ    | 100 | LYS  |
| 18  | QR    | 27  | GLY  |
| 18  | QR    | 54  | ARG  |
| 18  | QR    | 64  | ARG  |
| 18  | QR    | 65  | ILE  |
| 19  | QS    | 13  | ASP  |
| 19  | QS    | 45  | VAL  |
| 20  | QT    | 11  | SER  |
| 20  | QT    | 28  | ALA  |
| 20  | QT    | 62  | LEU  |
| 20  | QT    | 99  | LEU  |
| 20  | QT    | 102 | GLY  |
| 20  | QT    | 103 | GLY  |
| 21  | QU    | 3   | LYS  |
| 27  | RD    | 3   | VAL  |
| 27  | RD    | 32  | SER  |
| 27  | RD    | 58  | HIS  |
| 27  | RD    | 122 | ASP  |
| 27  | RD    | 169 | GLU  |
| 28  | RE    | 8   | LYS  |
| 28  | RE    | 20  | ALA  |
| 28  | RE    | 37  | ARG  |
| 28  | RE    | 53  | PRO  |
| 28  | RE    | 61  | ARG  |
| 28  | RE    | 78  | LEU  |
| 28  | RE    | 88  | GLY  |
| 28  | RE    | 186 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | RE    | 190 | GLY  |
| 28  | RE    | 204 | ALA  |
| 29  | RF    | 18  | ARG  |
| 29  | RF    | 107 | LYS  |
| 29  | RF    | 108 | LYS  |
| 29  | RF    | 111 | ALA  |
| 29  | RF    | 132 | VAL  |
| 29  | RF    | 134 | GLY  |
| 29  | RF    | 168 | ARG  |
| 30  | RG    | 36  | LYS  |
| 30  | RG    | 81  | LYS  |
| 30  | RG    | 82  | LEU  |
| 30  | RG    | 96  | ARG  |
| 30  | RG    | 110 | ALA  |
| 30  | RG    | 126 | ASP  |
| 30  | RG    | 136 | ARG  |
| 31  | RH    | 3   | ARG  |
| 31  | RH    | 8   | PRO  |
| 31  | RH    | 55  | PRO  |
| 31  | RH    | 59  | ARG  |
| 31  | RH    | 84  | SER  |
| 31  | RH    | 151 | ILE  |
| 31  | RH    | 156 | ALA  |
| 31  | RH    | 168 | PRO  |
| 32  | RI    | 13  | GLY  |
| 32  | RI    | 117 | GLU  |
| 32  | RI    | 133 | HIS  |
| 32  | RI    | 145 | VAL  |
| 33  | RN    | 23  | LEU  |
| 33  | RN    | 76  | SER  |
| 34  | RO    | 51  | ALA  |
| 34  | RO    | 56  | ASP  |
| 34  | RO    | 68  | GLU  |
| 35  | RP    | 6   | LEU  |
| 35  | RP    | 11  | GLY  |
| 35  | RP    | 12  | ALA  |
| 35  | RP    | 16  | ARG  |
| 36  | RQ    | 13  | GLN  |
| 36  | RQ    | 24  | GLY  |
| 36  | RQ    | 28  | ALA  |
| 36  | RQ    | 57  | HIS  |
| 37  | RR    | 11  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | RS    | 87  | PHE  |
| 38  | RS    | 96  | GLY  |
| 38  | RS    | 100 | ALA  |
| 38  | RS    | 109 | GLY  |
| 38  | RS    | 111 | GLU  |
| 39  | RT    | 4   | GLY  |
| 39  | RT    | 36  | GLU  |
| 39  | RT    | 43  | GLN  |
| 39  | RT    | 67  | SER  |
| 39  | RT    | 124 | ASP  |
| 40  | RU    | 9   | VAL  |
| 40  | RU    | 28  | ARG  |
| 40  | RU    | 73  | GLY  |
| 40  | RU    | 90  | VAL  |
| 42  | RW    | 63  | ASP  |
| 42  | RW    | 66  | GLU  |
| 43  | RX    | 67  | GLY  |
| 44  | RY    | 41  | GLY  |
| 44  | RY    | 56  | PRO  |
| 44  | RY    | 57  | GLN  |
| 44  | RY    | 91  | GLU  |
| 44  | RY    | 99  | CYS  |
| 45  | RZ    | 108 | PRO  |
| 45  | RZ    | 177 | PRO  |
| 47  | R1    | 45  | ASN  |
| 47  | R1    | 55  | GLY  |
| 47  | R1    | 84  | GLY  |
| 48  | R2    | 24  | LEU  |
| 48  | R2    | 44  | LEU  |
| 48  | R2    | 70  | GLN  |
| 50  | R4    | 9   | LEU  |
| 50  | R4    | 24  | THR  |
| 51  | R5    | 43  | HIS  |
| 51  | R5    | 55  | ARG  |
| 53  | R7    | 39  | ARG  |
| 2   | XB    | 18  | GLY  |
| 2   | XB    | 65  | GLY  |
| 2   | XB    | 208 | ILE  |
| 2   | XB    | 216 | SER  |
| 2   | XB    | 237 | ALA  |
| 3   | XC    | 60  | ALA  |
| 3   | XC    | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | XC    | 129 | ALA  |
| 3   | XC    | 145 | GLY  |
| 4   | XD    | 7   | PRO  |
| 4   | XD    | 20  | TYR  |
| 4   | XD    | 32  | ALA  |
| 4   | XD    | 164 | ALA  |
| 4   | XD    | 170 | VAL  |
| 4   | XD    | 179 | GLU  |
| 4   | XD    | 181 | MET  |
| 4   | XD    | 200 | GLU  |
| 5   | XE    | 21  | ALA  |
| 5   | XE    | 63  | ARG  |
| 5   | XE    | 108 | ALA  |
| 6   | XF    | 70  | ASP  |
| 7   | XG    | 4   | ARG  |
| 7   | XG    | 63  | LYS  |
| 7   | XG    | 141 | VAL  |
| 8   | XH    | 68  | ARG  |
| 8   | XH    | 69  | ARG  |
| 8   | XH    | 76  | PRO  |
| 8   | XH    | 122 | ARG  |
| 9   | XI    | 31  | GLN  |
| 9   | XI    | 41  | VAL  |
| 9   | XI    | 100 | GLY  |
| 9   | XI    | 109 | VAL  |
| 10  | XJ    | 36  | GLY  |
| 10  | XJ    | 68  | HIS  |
| 11  | XK    | 103 | LEU  |
| 11  | XK    | 107 | SER  |
| 11  | XK    | 124 | LYS  |
| 11  | XK    | 125 | PHE  |
| 11  | XK    | 126 | ARG  |
| 12  | XL    | 65  | GLU  |
| 12  | XL    | 110 | VAL  |
| 12  | XL    | 115 | LYS  |
| 12  | XL    | 116 | SER  |
| 12  | XL    | 128 | ALA  |
| 13  | XM    | 49  | THR  |
| 13  | XM    | 68  | GLY  |
| 13  | XM    | 118 | ALA  |
| 13  | XM    | 120 | LYS  |
| 14  | XN    | 14  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | XN    | 15  | LYS  |
| 14  | XN    | 40  | CYS  |
| 15  | XO    | 77  | ARG  |
| 16  | XP    | 49  | LEU  |
| 17  | XQ    | 14  | LYS  |
| 17  | XQ    | 33  | GLY  |
| 17  | XQ    | 78  | GLU  |
| 17  | XQ    | 100 | LYS  |
| 18  | XR    | 27  | GLY  |
| 18  | XR    | 54  | ARG  |
| 18  | XR    | 64  | ARG  |
| 18  | XR    | 65  | ILE  |
| 19  | XS    | 13  | ASP  |
| 19  | XS    | 45  | VAL  |
| 20  | XT    | 11  | SER  |
| 20  | XT    | 28  | ALA  |
| 20  | XT    | 62  | LEU  |
| 20  | XT    | 99  | LEU  |
| 20  | XT    | 102 | GLY  |
| 20  | XT    | 103 | GLY  |
| 21  | XU    | 3   | LYS  |
| 27  | YD    | 3   | VAL  |
| 27  | YD    | 32  | SER  |
| 27  | YD    | 58  | HIS  |
| 27  | YD    | 122 | ASP  |
| 27  | YD    | 169 | GLU  |
| 28  | YE    | 8   | LYS  |
| 28  | YE    | 20  | ALA  |
| 28  | YE    | 37  | ARG  |
| 28  | YE    | 53  | PRO  |
| 28  | YE    | 61  | ARG  |
| 28  | YE    | 71  | GLY  |
| 28  | YE    | 78  | LEU  |
| 28  | YE    | 88  | GLY  |
| 28  | YE    | 186 | GLY  |
| 28  | YE    | 190 | GLY  |
| 28  | YE    | 204 | ALA  |
| 29  | YF    | 18  | ARG  |
| 29  | YF    | 107 | LYS  |
| 29  | YF    | 108 | LYS  |
| 29  | YF    | 111 | ALA  |
| 29  | YF    | 132 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | YF    | 134 | GLY  |
| 29  | YF    | 168 | ARG  |
| 30  | YG    | 36  | LYS  |
| 30  | YG    | 81  | LYS  |
| 30  | YG    | 82  | LEU  |
| 30  | YG    | 96  | ARG  |
| 30  | YG    | 110 | ALA  |
| 30  | YG    | 115 | ARG  |
| 30  | YG    | 126 | ASP  |
| 30  | YG    | 136 | ARG  |
| 31  | YH    | 3   | ARG  |
| 31  | YH    | 8   | PRO  |
| 31  | YH    | 55  | PRO  |
| 31  | YH    | 59  | ARG  |
| 31  | YH    | 84  | SER  |
| 31  | YH    | 151 | ILE  |
| 31  | YH    | 156 | ALA  |
| 31  | YH    | 168 | PRO  |
| 32  | YI    | 11  | ASN  |
| 32  | YI    | 84  | GLY  |
| 32  | YI    | 114 | LEU  |
| 33  | YN    | 23  | LEU  |
| 33  | YN    | 76  | SER  |
| 34  | YO    | 51  | ALA  |
| 34  | YO    | 56  | ASP  |
| 34  | YO    | 68  | GLU  |
| 35  | YP    | 6   | LEU  |
| 35  | YP    | 11  | GLY  |
| 35  | YP    | 12  | ALA  |
| 35  | YP    | 16  | ARG  |
| 36  | YQ    | 13  | GLN  |
| 36  | YQ    | 24  | GLY  |
| 36  | YQ    | 28  | ALA  |
| 37  | YR    | 11  | ASN  |
| 38  | YS    | 61  | ASN  |
| 38  | YS    | 87  | PHE  |
| 38  | YS    | 96  | GLY  |
| 38  | YS    | 100 | ALA  |
| 38  | YS    | 109 | GLY  |
| 38  | YS    | 111 | GLU  |
| 39  | YT    | 4   | GLY  |
| 39  | YT    | 36  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | YT    | 43  | GLN  |
| 39  | YT    | 67  | SER  |
| 39  | YT    | 124 | ASP  |
| 40  | YU    | 9   | VAL  |
| 40  | YU    | 28  | ARG  |
| 40  | YU    | 73  | GLY  |
| 40  | YU    | 90  | VAL  |
| 42  | YW    | 63  | ASP  |
| 42  | YW    | 66  | GLU  |
| 43  | YX    | 67  | GLY  |
| 44  | YY    | 4   | LYS  |
| 44  | YY    | 41  | GLY  |
| 44  | YY    | 53  | PRO  |
| 44  | YY    | 56  | PRO  |
| 44  | YY    | 57  | GLN  |
| 44  | YY    | 99  | CYS  |
| 45  | YZ    | 59  | LEU  |
| 45  | YZ    | 113 | ALA  |
| 47  | Y1    | 45  | ASN  |
| 47  | Y1    | 55  | GLY  |
| 47  | Y1    | 84  | GLY  |
| 48  | Y2    | 24  | LEU  |
| 48  | Y2    | 44  | LEU  |
| 48  | Y2    | 70  | GLN  |
| 50  | Y4    | 9   | LEU  |
| 50  | Y4    | 24  | THR  |
| 51  | Y5    | 43  | HIS  |
| 51  | Y5    | 55  | ARG  |
| 53  | Y7    | 39  | ARG  |
| 2   | QB    | 155 | LEU  |
| 2   | QB    | 159 | PRO  |
| 2   | QB    | 175 | ARG  |
| 3   | QC    | 16  | ARG  |
| 3   | QC    | 45  | LYS  |
| 3   | QC    | 81  | GLY  |
| 4   | QD    | 26  | CYS  |
| 4   | QD    | 136 | PRO  |
| 5   | QE    | 37  | ARG  |
| 5   | QE    | 124 | GLY  |
| 6   | QF    | 41  | GLU  |
| 6   | QF    | 87  | ARG  |
| 7   | QG    | 35  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | QG    | 62  | PHE  |
| 7   | QG    | 149 | ARG  |
| 8   | QH    | 2   | LEU  |
| 9   | QI    | 12  | GLU  |
| 9   | QI    | 13  | ALA  |
| 10  | QJ    | 57  | LYS  |
| 12  | QL    | 51  | ALA  |
| 12  | QL    | 123 | LYS  |
| 13  | QM    | 12  | ASN  |
| 13  | QM    | 101 | GLN  |
| 13  | QM    | 121 | LYS  |
| 14  | QN    | 9   | LYS  |
| 15  | QO    | 14  | GLU  |
| 15  | QO    | 23  | GLY  |
| 16  | QP    | 8   | ARG  |
| 16  | QP    | 83  | GLU  |
| 17  | QQ    | 30  | PRO  |
| 17  | QQ    | 99  | SER  |
| 18  | QR    | 55  | ARG  |
| 19  | QS    | 6   | LYS  |
| 19  | QS    | 27  | GLU  |
| 19  | QS    | 64  | GLU  |
| 20  | QT    | 82  | SER  |
| 20  | QT    | 98  | PRO  |
| 27  | RD    | 111 | LEU  |
| 27  | RD    | 242 | ARG  |
| 27  | RD    | 262 | ARG  |
| 28  | RE    | 62  | PRO  |
| 28  | RE    | 69  | LYS  |
| 28  | RE    | 71  | GLY  |
| 28  | RE    | 82  | ARG  |
| 28  | RE    | 117 | MET  |
| 28  | RE    | 130 | GLY  |
| 28  | RE    | 132 | HIS  |
| 30  | RG    | 5   | VAL  |
| 30  | RG    | 115 | ARG  |
| 30  | RG    | 128 | ARG  |
| 30  | RG    | 174 | GLU  |
| 31  | RH    | 50  | VAL  |
| 31  | RH    | 81  | GLU  |
| 31  | RH    | 152 | ARG  |
| 32  | RI    | 11  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | RI    | 118 | LYS  |
| 33  | RN    | 45  | ASN  |
| 33  | RN    | 130 | HIS  |
| 33  | RN    | 132 | ALA  |
| 33  | RN    | 135 | PRO  |
| 35  | RP    | 7   | ARG  |
| 35  | RP    | 14  | LYS  |
| 35  | RP    | 43  | GLY  |
| 35  | RP    | 89  | ALA  |
| 35  | RP    | 102 | ARG  |
| 35  | RP    | 115 | LEU  |
| 36  | RQ    | 88  | GLY  |
| 36  | RQ    | 91  | GLU  |
| 37  | RR    | 42  | LYS  |
| 37  | RR    | 45  | ARG  |
| 37  | RR    | 71  | GLN  |
| 37  | RR    | 107 | ASP  |
| 38  | RS    | 19  | LYS  |
| 38  | RS    | 61  | ASN  |
| 38  | RS    | 74  | ALA  |
| 38  | RS    | 75  | GLU  |
| 39  | RT    | 78  | LEU  |
| 39  | RT    | 112 | ARG  |
| 40  | RU    | 46  | ALA  |
| 40  | RU    | 58  | ARG  |
| 40  | RU    | 93  | LYS  |
| 41  | RV    | 54  | GLY  |
| 42  | RW    | 68  | ARG  |
| 42  | RW    | 93  | ALA  |
| 43  | RX    | 48  | LYS  |
| 43  | RX    | 87  | GLN  |
| 44  | RY    | 21  | LYS  |
| 44  | RY    | 39  | VAL  |
| 44  | RY    | 42  | VAL  |
| 44  | RY    | 69  | ALA  |
| 44  | RY    | 102 | CYS  |
| 45  | RZ    | 59  | LEU  |
| 45  | RZ    | 112 | ARG  |
| 45  | RZ    | 116 | VAL  |
| 47  | R1    | 74  | VAL  |
| 47  | R1    | 91  | LYS  |
| 47  | R1    | 93  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | R4    | 27  | THR  |
| 50  | R4    | 46  | GLN  |
| 52  | R6    | 18  | ARG  |
| 53  | R7    | 32  | LYS  |
| 54  | R8    | 46  | ARG  |
| 54  | R8    | 47  | LYS  |
| 2   | XB    | 155 | LEU  |
| 2   | XB    | 159 | PRO  |
| 3   | XC    | 16  | ARG  |
| 3   | XC    | 45  | LYS  |
| 3   | XC    | 81  | GLY  |
| 4   | XD    | 29  | PRO  |
| 4   | XD    | 73  | ARG  |
| 4   | XD    | 136 | PRO  |
| 5   | XE    | 37  | ARG  |
| 6   | XF    | 41  | GLU  |
| 6   | XF    | 87  | ARG  |
| 7   | XG    | 62  | PHE  |
| 7   | XG    | 149 | ARG  |
| 8   | XH    | 2   | LEU  |
| 8   | XH    | 128 | GLY  |
| 9   | XI    | 12  | GLU  |
| 9   | XI    | 13  | ALA  |
| 10  | XJ    | 57  | LYS  |
| 12  | XL    | 51  | ALA  |
| 12  | XL    | 123 | LYS  |
| 13  | XM    | 12  | ASN  |
| 13  | XM    | 101 | GLN  |
| 13  | XM    | 121 | LYS  |
| 14  | XN    | 9   | LYS  |
| 14  | XN    | 48  | ALA  |
| 15  | XO    | 14  | GLU  |
| 15  | XO    | 23  | GLY  |
| 16  | XP    | 8   | ARG  |
| 16  | XP    | 83  | GLU  |
| 17  | XQ    | 30  | PRO  |
| 17  | XQ    | 99  | SER  |
| 18  | XR    | 55  | ARG  |
| 19  | XS    | 6   | LYS  |
| 19  | XS    | 27  | GLU  |
| 20  | XT    | 82  | SER  |
| 20  | XT    | 98  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | YD    | 12  | SER  |
| 27  | YD    | 111 | LEU  |
| 27  | YD    | 239 | ARG  |
| 27  | YD    | 242 | ARG  |
| 27  | YD    | 262 | ARG  |
| 28  | YE    | 62  | PRO  |
| 28  | YE    | 69  | LYS  |
| 28  | YE    | 82  | ARG  |
| 28  | YE    | 117 | MET  |
| 28  | YE    | 130 | GLY  |
| 28  | YE    | 132 | HIS  |
| 30  | YG    | 5   | VAL  |
| 30  | YG    | 128 | ARG  |
| 30  | YG    | 174 | GLU  |
| 31  | YH    | 50  | VAL  |
| 31  | YH    | 81  | GLU  |
| 31  | YH    | 152 | ARG  |
| 32  | YI    | 13  | GLY  |
| 32  | YI    | 72  | LEU  |
| 32  | YI    | 113 | ARG  |
| 32  | YI    | 118 | LYS  |
| 33  | YN    | 45  | ASN  |
| 33  | YN    | 130 | HIS  |
| 33  | YN    | 135 | PRO  |
| 35  | YP    | 7   | ARG  |
| 35  | YP    | 14  | LYS  |
| 35  | YP    | 43  | GLY  |
| 35  | YP    | 89  | ALA  |
| 35  | YP    | 102 | ARG  |
| 35  | YP    | 115 | LEU  |
| 36  | YQ    | 57  | HIS  |
| 36  | YQ    | 88  | GLY  |
| 36  | YQ    | 91  | GLU  |
| 37  | YR    | 42  | LYS  |
| 37  | YR    | 45  | ARG  |
| 37  | YR    | 71  | GLN  |
| 37  | YR    | 107 | ASP  |
| 38  | YS    | 19  | LYS  |
| 38  | YS    | 74  | ALA  |
| 38  | YS    | 75  | GLU  |
| 39  | YT    | 78  | LEU  |
| 39  | YT    | 112 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | YU    | 46  | ALA  |
| 40  | YU    | 58  | ARG  |
| 40  | YU    | 93  | LYS  |
| 41  | YV    | 54  | GLY  |
| 42  | YW    | 68  | ARG  |
| 42  | YW    | 93  | ALA  |
| 43  | YX    | 48  | LYS  |
| 43  | YX    | 87  | GLN  |
| 44  | YY    | 21  | LYS  |
| 44  | YY    | 39  | VAL  |
| 44  | YY    | 42  | VAL  |
| 44  | YY    | 69  | ALA  |
| 44  | YY    | 91  | GLU  |
| 44  | YY    | 102 | CYS  |
| 45  | YZ    | 13  | GLU  |
| 45  | YZ    | 81  | ARG  |
| 47  | Y1    | 74  | VAL  |
| 47  | Y1    | 91  | LYS  |
| 47  | Y1    | 93  | GLU  |
| 50  | Y4    | 27  | THR  |
| 50  | Y4    | 46  | GLN  |
| 52  | Y6    | 18  | ARG  |
| 53  | Y7    | 32  | LYS  |
| 54  | Y8    | 46  | ARG  |
| 54  | Y8    | 47  | LYS  |
| 2   | QB    | 19  | HIS  |
| 2   | QB    | 131 | PRO  |
| 2   | QB    | 160 | ASP  |
| 2   | QB    | 177 | ALA  |
| 3   | QC    | 168 | ALA  |
| 4   | QD    | 151 | LYS  |
| 5   | QE    | 70  | PRO  |
| 5   | QE    | 72  | GLN  |
| 6   | QF    | 13  | ASN  |
| 6   | QF    | 40  | VAL  |
| 6   | QF    | 42  | GLU  |
| 7   | QG    | 41  | ARG  |
| 7   | QG    | 109 | ASN  |
| 7   | QG    | 116 | ALA  |
| 7   | QG    | 117 | ALA  |
| 8   | QH    | 27  | PRO  |
| 8   | QH    | 49  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | QJ    | 93  | GLY  |
| 12  | QL    | 64  | TYR  |
| 13  | QM    | 4   | ILE  |
| 13  | QM    | 14  | ARG  |
| 13  | QM    | 69  | GLU  |
| 13  | QM    | 77  | ASN  |
| 14  | QN    | 26  | ARG  |
| 14  | QN    | 48  | ALA  |
| 15  | QO    | 86  | GLY  |
| 16  | QP    | 26  | ARG  |
| 16  | QP    | 28  | ARG  |
| 16  | QP    | 48  | TRP  |
| 19  | QS    | 28  | LYS  |
| 19  | QS    | 44  | MET  |
| 20  | QT    | 40  | ALA  |
| 20  | QT    | 51  | GLU  |
| 27  | RD    | 12  | SER  |
| 27  | RD    | 73  | VAL  |
| 27  | RD    | 238 | GLY  |
| 28  | RE    | 66  | HIS  |
| 28  | RE    | 126 | PRO  |
| 29  | RF    | 43  | LYS  |
| 29  | RF    | 130 | ALA  |
| 29  | RF    | 145 | GLU  |
| 30  | RG    | 12  | TYR  |
| 30  | RG    | 117 | PHE  |
| 30  | RG    | 146 | TYR  |
| 31  | RH    | 13  | LYS  |
| 31  | RH    | 109 | PHE  |
| 31  | RH    | 159 | GLU  |
| 32  | RI    | 72  | LEU  |
| 33  | RN    | 96  | GLU  |
| 33  | RN    | 127 | ASP  |
| 34  | RO    | 17  | ARG  |
| 34  | RO    | 97  | ARG  |
| 35  | RP    | 29  | LYS  |
| 35  | RP    | 47  | ASP  |
| 35  | RP    | 139 | LYS  |
| 39  | RT    | 37  | GLY  |
| 39  | RT    | 95  | ARG  |
| 40  | RU    | 74  | LEU  |
| 42  | RW    | 14  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | RW    | 48  | ALA  |
| 45  | RZ    | 61  | LEU  |
| 45  | RZ    | 166 | SER  |
| 46  | R0    | 3   | HIS  |
| 46  | R0    | 18  | ALA  |
| 50  | R4    | 8   | LYS  |
| 51  | R5    | 14  | ALA  |
| 51  | R5    | 37  | LYS  |
| 51  | R5    | 45  | VAL  |
| 51  | R5    | 48  | GLU  |
| 52  | R6    | 8   | LYS  |
| 52  | R6    | 9   | LEU  |
| 52  | R6    | 10  | LEU  |
| 52  | R6    | 49  | HIS  |
| 54  | R8    | 25  | MET  |
| 54  | R8    | 53  | PRO  |
| 54  | R8    | 57  | ARG  |
| 2   | XB    | 19  | HIS  |
| 2   | XB    | 131 | PRO  |
| 2   | XB    | 160 | ASP  |
| 2   | XB    | 175 | ARG  |
| 3   | XC    | 168 | ALA  |
| 4   | XD    | 151 | LYS  |
| 5   | XE    | 70  | PRO  |
| 5   | XE    | 72  | GLN  |
| 5   | XE    | 124 | GLY  |
| 6   | XF    | 13  | ASN  |
| 6   | XF    | 40  | VAL  |
| 6   | XF    | 42  | GLU  |
| 7   | XG    | 35  | LYS  |
| 7   | XG    | 41  | ARG  |
| 7   | XG    | 116 | ALA  |
| 7   | XG    | 117 | ALA  |
| 8   | XH    | 27  | PRO  |
| 8   | XH    | 29  | SER  |
| 8   | XH    | 49  | GLU  |
| 10  | XJ    | 93  | GLY  |
| 12  | XL    | 64  | TYR  |
| 13  | XM    | 4   | ILE  |
| 13  | XM    | 14  | ARG  |
| 13  | XM    | 69  | GLU  |
| 13  | XM    | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | XN    | 22  | THR  |
| 15  | XO    | 86  | GLY  |
| 16  | XP    | 26  | ARG  |
| 16  | XP    | 28  | ARG  |
| 16  | XP    | 48  | TRP  |
| 19  | XS    | 28  | LYS  |
| 19  | XS    | 44  | MET  |
| 19  | XS    | 64  | GLU  |
| 20  | XT    | 40  | ALA  |
| 20  | XT    | 51  | GLU  |
| 27  | YD    | 73  | VAL  |
| 28  | YE    | 66  | HIS  |
| 28  | YE    | 126 | PRO  |
| 29  | YF    | 43  | LYS  |
| 29  | YF    | 130 | ALA  |
| 29  | YF    | 136 | THR  |
| 29  | YF    | 145 | GLU  |
| 30  | YG    | 12  | TYR  |
| 30  | YG    | 117 | PHE  |
| 30  | YG    | 146 | TYR  |
| 31  | YH    | 13  | LYS  |
| 31  | YH    | 109 | PHE  |
| 31  | YH    | 159 | GLU  |
| 32  | YI    | 87  | LYS  |
| 32  | YI    | 102 | SER  |
| 33  | YN    | 96  | GLU  |
| 33  | YN    | 127 | ASP  |
| 33  | YN    | 132 | ALA  |
| 34  | YO    | 17  | ARG  |
| 34  | YO    | 97  | ARG  |
| 35  | YP    | 29  | LYS  |
| 35  | YP    | 47  | ASP  |
| 35  | YP    | 139 | LYS  |
| 39  | YT    | 37  | GLY  |
| 39  | YT    | 95  | ARG  |
| 40  | YU    | 74  | LEU  |
| 42  | YW    | 14  | PRO  |
| 42  | YW    | 48  | ALA  |
| 45  | YZ    | 6   | LYS  |
| 45  | YZ    | 51  | ALA  |
| 45  | YZ    | 181 | GLU  |
| 50  | Y4    | 8   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | Y5    | 14  | ALA  |
| 51  | Y5    | 37  | LYS  |
| 51  | Y5    | 45  | VAL  |
| 51  | Y5    | 48  | GLU  |
| 52  | Y6    | 8   | LYS  |
| 52  | Y6    | 9   | LEU  |
| 52  | Y6    | 10  | LEU  |
| 52  | Y6    | 49  | HIS  |
| 54  | Y8    | 25  | MET  |
| 54  | Y8    | 53  | PRO  |
| 2   | QB    | 23  | ARG  |
| 2   | QB    | 25  | ASN  |
| 2   | QB    | 98  | LEU  |
| 2   | QB    | 129 | GLU  |
| 2   | QB    | 194 | PRO  |
| 2   | QB    | 229 | VAL  |
| 2   | QB    | 231 | GLU  |
| 3   | QC    | 125 | GLU  |
| 5   | QE    | 74  | GLY  |
| 5   | QE    | 77  | PRO  |
| 5   | QE    | 112 | LEU  |
| 5   | QE    | 128 | PRO  |
| 5   | QE    | 132 | ALA  |
| 6   | QF    | 12  | PRO  |
| 6   | QF    | 32  | ASN  |
| 6   | QF    | 96  | PRO  |
| 8   | QH    | 29  | SER  |
| 8   | QH    | 34  | GLU  |
| 8   | QH    | 103 | VAL  |
| 9   | QI    | 44  | VAL  |
| 9   | QI    | 88  | TYR  |
| 9   | QI    | 89  | ASN  |
| 10  | QJ    | 53  | PRO  |
| 10  | QJ    | 59  | SER  |
| 10  | QJ    | 75  | ILE  |
| 11  | QK    | 64  | ALA  |
| 11  | QK    | 105 | VAL  |
| 12  | QL    | 63  | GLY  |
| 18  | QR    | 58  | LEU  |
| 19  | QS    | 11  | VAL  |
| 27  | RD    | 33  | LEU  |
| 28  | RE    | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | RF    | 47  | GLY  |
| 29  | RF    | 118 | ALA  |
| 29  | RF    | 136 | THR  |
| 30  | RG    | 181 | ARG  |
| 31  | RH    | 11  | VAL  |
| 31  | RH    | 27  | LYS  |
| 31  | RH    | 47  | GLU  |
| 31  | RH    | 77  | LYS  |
| 31  | RH    | 170 | ARG  |
| 33  | RN    | 29  | LYS  |
| 33  | RN    | 104 | LYS  |
| 33  | RN    | 128 | HIS  |
| 34  | RO    | 25  | LEU  |
| 35  | RP    | 50  | ARG  |
| 35  | RP    | 97  | PRO  |
| 35  | RP    | 108 | LYS  |
| 37  | RR    | 85  | PRO  |
| 40  | RU    | 91  | ASP  |
| 42  | RW    | 32  | ALA  |
| 44  | RY    | 7   | VAL  |
| 45  | RZ    | 13  | GLU  |
| 45  | RZ    | 62  | PRO  |
| 49  | R3    | 13  | ILE  |
| 50  | R4    | 30  | GLU  |
| 50  | R4    | 33  | VAL  |
| 51  | R5    | 42  | PRO  |
| 52  | R6    | 35  | GLU  |
| 54  | R8    | 64  | TYR  |
| 2   | XB    | 23  | ARG  |
| 2   | XB    | 98  | LEU  |
| 2   | XB    | 129 | GLU  |
| 2   | XB    | 177 | ALA  |
| 2   | XB    | 194 | PRO  |
| 2   | XB    | 229 | VAL  |
| 2   | XB    | 231 | GLU  |
| 3   | XC    | 125 | GLU  |
| 5   | XE    | 74  | GLY  |
| 5   | XE    | 77  | PRO  |
| 5   | XE    | 112 | LEU  |
| 5   | XE    | 128 | PRO  |
| 5   | XE    | 132 | ALA  |
| 6   | XF    | 12  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | XF    | 32  | ASN  |
| 6   | XF    | 96  | PRO  |
| 7   | XG    | 109 | ASN  |
| 8   | XH    | 34  | GLU  |
| 8   | XH    | 103 | VAL  |
| 9   | XI    | 44  | VAL  |
| 9   | XI    | 88  | TYR  |
| 9   | XI    | 89  | ASN  |
| 10  | XJ    | 53  | PRO  |
| 10  | XJ    | 59  | SER  |
| 10  | XJ    | 75  | ILE  |
| 11  | XK    | 64  | ALA  |
| 11  | XK    | 105 | VAL  |
| 12  | XL    | 63  | GLY  |
| 14  | XN    | 20  | ALA  |
| 18  | XR    | 58  | LEU  |
| 19  | XS    | 11  | VAL  |
| 27  | YD    | 33  | LEU  |
| 28  | YE    | 79  | ARG  |
| 29  | YF    | 47  | GLY  |
| 29  | YF    | 118 | ALA  |
| 31  | YH    | 11  | VAL  |
| 31  | YH    | 27  | LYS  |
| 31  | YH    | 47  | GLU  |
| 31  | YH    | 77  | LYS  |
| 31  | YH    | 170 | ARG  |
| 32  | YI    | 12  | LEU  |
| 32  | YI    | 15  | VAL  |
| 32  | YI    | 18  | VAL  |
| 32  | YI    | 122 | GLU  |
| 33  | YN    | 29  | LYS  |
| 33  | YN    | 104 | LYS  |
| 33  | YN    | 128 | HIS  |
| 34  | YO    | 25  | LEU  |
| 35  | YP    | 50  | ARG  |
| 35  | YP    | 97  | PRO  |
| 35  | YP    | 108 | LYS  |
| 37  | YR    | 85  | PRO  |
| 40  | YU    | 91  | ASP  |
| 42  | YW    | 32  | ALA  |
| 43  | YX    | 19  | ALA  |
| 44  | YY    | 7   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | YZ    | 53  | ILE  |
| 45  | YZ    | 61  | LEU  |
| 45  | YZ    | 92  | SER  |
| 49  | Y3    | 13  | ILE  |
| 50  | Y4    | 30  | GLU  |
| 50  | Y4    | 33  | VAL  |
| 50  | Y4    | 70  | GLY  |
| 51  | Y5    | 42  | PRO  |
| 52  | Y6    | 35  | GLU  |
| 53  | Y7    | 44  | PRO  |
| 54  | Y8    | 57  | ARG  |
| 54  | Y8    | 64  | TYR  |
| 3   | QC    | 51  | GLY  |
| 5   | QE    | 115 | VAL  |
| 13  | QM    | 48  | LEU  |
| 14  | QN    | 20  | ALA  |
| 16  | QP    | 57  | ARG  |
| 20  | QT    | 70  | SER  |
| 27  | RD    | 178 | PRO  |
| 30  | RG    | 109 | VAL  |
| 31  | RH    | 7   | LEU  |
| 31  | RH    | 26  | VAL  |
| 32  | RI    | 18  | VAL  |
| 32  | RI    | 102 | SER  |
| 32  | RI    | 122 | GLU  |
| 39  | RT    | 38  | ASN  |
| 42  | RW    | 11  | ARG  |
| 42  | RW    | 33  | ARG  |
| 43  | RX    | 19  | ALA  |
| 45  | RZ    | 66  | SER  |
| 50  | R4    | 69  | LYS  |
| 50  | R4    | 70  | GLY  |
| 51  | R5    | 57  | VAL  |
| 53  | R7    | 44  | PRO  |
| 2   | XB    | 25  | ASN  |
| 3   | XC    | 51  | GLY  |
| 5   | XE    | 49  | PRO  |
| 5   | XE    | 115 | VAL  |
| 10  | XJ    | 85  | LEU  |
| 11  | XK    | 106 | LYS  |
| 13  | XM    | 109 | THR  |
| 16  | XP    | 57  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | XT    | 70  | SER  |
| 27  | YD    | 178 | PRO  |
| 27  | YD    | 241 | PRO  |
| 30  | YG    | 109 | VAL  |
| 30  | YG    | 181 | ARG  |
| 31  | YH    | 7   | LEU  |
| 31  | YH    | 26  | VAL  |
| 39  | YT    | 38  | ASN  |
| 41  | YV    | 36  | PRO  |
| 42  | YW    | 11  | ARG  |
| 42  | YW    | 33  | ARG  |
| 45  | YZ    | 168 | GLU  |
| 45  | YZ    | 177 | PRO  |
| 50  | Y4    | 69  | LYS  |
| 51  | Y5    | 57  | VAL  |
| 2   | QB    | 202 | PRO  |
| 2   | QB    | 239 | VAL  |
| 4   | QD    | 88  | VAL  |
| 5   | QE    | 49  | PRO  |
| 7   | QG    | 55  | GLY  |
| 7   | QG    | 58  | PRO  |
| 8   | QH    | 106 | GLY  |
| 18  | QR    | 37  | VAL  |
| 20  | QT    | 63  | ILE  |
| 28  | RE    | 86  | PRO  |
| 28  | RE    | 184 | VAL  |
| 36  | RQ    | 86  | GLY  |
| 37  | RR    | 32  | GLY  |
| 41  | RV    | 36  | PRO  |
| 42  | RW    | 35  | ILE  |
| 45  | RZ    | 141 | VAL  |
| 46  | R0    | 8   | GLY  |
| 2   | XB    | 202 | PRO  |
| 2   | XB    | 239 | VAL  |
| 4   | XD    | 88  | VAL  |
| 7   | XG    | 55  | GLY  |
| 7   | XG    | 58  | PRO  |
| 15  | XO    | 18  | PHE  |
| 18  | XR    | 37  | VAL  |
| 20  | XT    | 63  | ILE  |
| 28  | YE    | 86  | PRO  |
| 28  | YE    | 184 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | YQ    | 86  | GLY  |
| 37  | YR    | 32  | GLY  |
| 42  | YW    | 35  | ILE  |
| 51  | Y5    | 46  | CYS  |
| 2   | QB    | 227 | GLY  |
| 3   | QC    | 114 | PRO  |
| 4   | QD    | 90  | GLY  |
| 9   | QI    | 24  | GLY  |
| 13  | QM    | 60  | VAL  |
| 15  | QO    | 18  | PHE  |
| 16  | QP    | 53  | VAL  |
| 27  | RD    | 241 | PRO  |
| 44  | RY    | 27  | VAL  |
| 44  | RY    | 32  | PRO  |
| 45  | RZ    | 106 | GLY  |
| 51  | R5    | 46  | CYS  |
| 2   | XB    | 227 | GLY  |
| 3   | XC    | 114 | PRO  |
| 4   | XD    | 90  | GLY  |
| 8   | XH    | 106 | GLY  |
| 9   | XI    | 24  | GLY  |
| 13  | XM    | 60  | VAL  |
| 16  | XP    | 53  | VAL  |
| 30  | YG    | 52  | ILE  |
| 44  | YY    | 27  | VAL  |
| 44  | YY    | 32  | PRO  |
| 45  | YZ    | 160 | GLY  |
| 3   | QC    | 134 | ILE  |
| 13  | QM    | 84  | ILE  |
| 27  | RD    | 34  | VAL  |
| 30  | RG    | 52  | ILE  |
| 32  | RI    | 15  | VAL  |
| 34  | RO    | 114 | ILE  |
| 44  | RY    | 51  | VAL  |
| 45  | RZ    | 165 | VAL  |
| 51  | R5    | 34  | PRO  |
| 3   | XC    | 134 | ILE  |
| 13  | XM    | 84  | ILE  |
| 27  | YD    | 34  | VAL  |
| 32  | YI    | 71  | ILE  |
| 34  | YO    | 114 | ILE  |
| 44  | YY    | 51  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | YZ    | 62  | PRO  |
| 51  | Y5    | 34  | PRO  |
| 9   | QI    | 21  | PRO  |
| 13  | QM    | 78  | ILE  |
| 28  | RE    | 52  | LEU  |
| 28  | RE    | 55  | ASN  |
| 34  | RO    | 27  | GLY  |
| 49  | R3    | 40  | THR  |
| 5   | XE    | 129 | ILE  |
| 9   | XI    | 21  | PRO  |
| 28  | YE    | 52  | LEU  |
| 28  | YE    | 55  | ASN  |
| 34  | YO    | 27  | GLY  |
| 49  | Y3    | 40  | THR  |
| 7   | QG    | 14  | PRO  |
| 8   | QH    | 51  | VAL  |
| 16  | QP    | 41  | PRO  |
| 20  | QT    | 97  | ALA  |
| 8   | XH    | 51  | VAL  |
| 13  | XM    | 78  | ILE  |
| 16  | XP    | 41  | PRO  |
| 20  | XT    | 97  | ALA  |
| 48  | R2    | 18  | PRO  |
| 48  | Y2    | 18  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | QB    | 205/220 (93%) | 182 (89%) | 23 (11%) | 6           | 25 |
| 2   | XB    | 205/220 (93%) | 181 (88%) | 24 (12%) | 5           | 24 |
| 3   | QC    | 159/188 (85%) | 142 (89%) | 17 (11%) | 6           | 27 |
| 3   | XC    | 159/188 (85%) | 142 (89%) | 17 (11%) | 6           | 27 |
| 4   | QD    | 180/181 (99%) | 156 (87%) | 24 (13%) | 4           | 20 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | XD    | 180/181 (99%)  | 162 (90%) | 18 (10%) | 7           | 29 |
| 5   | QE    | 116/123 (94%)  | 105 (90%) | 11 (10%) | 8           | 31 |
| 5   | XE    | 116/123 (94%)  | 105 (90%) | 11 (10%) | 8           | 31 |
| 6   | QF    | 90/90 (100%)   | 77 (86%)  | 13 (14%) | 3           | 18 |
| 6   | XF    | 90/90 (100%)   | 77 (86%)  | 13 (14%) | 3           | 18 |
| 7   | QG    | 126/127 (99%)  | 112 (89%) | 14 (11%) | 6           | 26 |
| 7   | XG    | 126/127 (99%)  | 112 (89%) | 14 (11%) | 6           | 26 |
| 8   | QH    | 119/119 (100%) | 105 (88%) | 14 (12%) | 5           | 23 |
| 8   | XH    | 119/119 (100%) | 105 (88%) | 14 (12%) | 5           | 23 |
| 9   | QI    | 98/99 (99%)    | 85 (87%)  | 13 (13%) | 4           | 20 |
| 9   | XI    | 98/99 (99%)    | 85 (87%)  | 13 (13%) | 4           | 20 |
| 10  | QJ    | 89/92 (97%)    | 80 (90%)  | 9 (10%)  | 7           | 28 |
| 10  | XJ    | 89/92 (97%)    | 80 (90%)  | 9 (10%)  | 7           | 28 |
| 11  | QK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 7           | 29 |
| 11  | XK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 7           | 29 |
| 12  | QL    | 104/109 (95%)  | 87 (84%)  | 17 (16%) | 2           | 14 |
| 12  | XL    | 104/109 (95%)  | 86 (83%)  | 18 (17%) | 2           | 12 |
| 13  | QM    | 97/101 (96%)   | 83 (86%)  | 14 (14%) | 3           | 18 |
| 13  | XM    | 97/101 (96%)   | 83 (86%)  | 14 (14%) | 3           | 18 |
| 14  | QN    | 49/50 (98%)    | 40 (82%)  | 9 (18%)  | 1           | 9  |
| 14  | XN    | 49/50 (98%)    | 44 (90%)  | 5 (10%)  | 7           | 28 |
| 15  | QO    | 79/80 (99%)    | 70 (89%)  | 9 (11%)  | 5           | 24 |
| 15  | XO    | 79/80 (99%)    | 70 (89%)  | 9 (11%)  | 5           | 24 |
| 16  | QP    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 6           | 26 |
| 16  | XP    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 6           | 26 |
| 17  | QQ    | 95/97 (98%)    | 86 (90%)  | 9 (10%)  | 8           | 31 |
| 17  | XQ    | 95/97 (98%)    | 86 (90%)  | 9 (10%)  | 8           | 31 |
| 18  | QR    | 61/77 (79%)    | 51 (84%)  | 10 (16%) | 2           | 14 |
| 18  | XR    | 61/77 (79%)    | 51 (84%)  | 10 (16%) | 2           | 14 |
| 19  | QS    | 73/80 (91%)    | 62 (85%)  | 11 (15%) | 3           | 16 |
| 19  | XS    | 73/80 (91%)    | 62 (85%)  | 11 (15%) | 3           | 16 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 20  | QT    | 76/82 (93%)    | 69 (91%)  | 7 (9%)   | 8           | 32  |
| 20  | XT    | 76/82 (93%)    | 69 (91%)  | 7 (9%)   | 8           | 32  |
| 21  | QU    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 21  | XU    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 27  | RD    | 214/218 (98%)  | 174 (81%) | 40 (19%) | 1           | 9   |
| 27  | YD    | 214/218 (98%)  | 174 (81%) | 40 (19%) | 1           | 9   |
| 28  | RE    | 165/166 (99%)  | 125 (76%) | 40 (24%) | 1           | 4   |
| 28  | YE    | 165/166 (99%)  | 125 (76%) | 40 (24%) | 1           | 4   |
| 29  | RF    | 161/166 (97%)  | 138 (86%) | 23 (14%) | 3           | 18  |
| 29  | YF    | 161/166 (97%)  | 138 (86%) | 23 (14%) | 3           | 18  |
| 30  | RG    | 155/156 (99%)  | 133 (86%) | 22 (14%) | 3           | 18  |
| 30  | YG    | 155/156 (99%)  | 134 (86%) | 21 (14%) | 4           | 20  |
| 31  | RH    | 142/148 (96%)  | 111 (78%) | 31 (22%) | 1           | 6   |
| 31  | YH    | 142/148 (96%)  | 111 (78%) | 31 (22%) | 1           | 6   |
| 32  | RI    | 122/124 (98%)  | 95 (78%)  | 27 (22%) | 1           | 5   |
| 32  | YI    | 122/124 (98%)  | 95 (78%)  | 27 (22%) | 1           | 5   |
| 33  | RN    | 117/119 (98%)  | 97 (83%)  | 20 (17%) | 2           | 12  |
| 33  | YN    | 117/119 (98%)  | 97 (83%)  | 20 (17%) | 2           | 12  |
| 34  | RO    | 100/100 (100%) | 89 (89%)  | 11 (11%) | 6           | 26  |
| 34  | YO    | 100/100 (100%) | 89 (89%)  | 11 (11%) | 6           | 26  |
| 35  | RP    | 116/116 (100%) | 88 (76%)  | 28 (24%) | 1           | 4   |
| 35  | YP    | 116/116 (100%) | 88 (76%)  | 28 (24%) | 1           | 4   |
| 36  | RQ    | 111/111 (100%) | 96 (86%)  | 15 (14%) | 4           | 20  |
| 36  | YQ    | 111/111 (100%) | 96 (86%)  | 15 (14%) | 4           | 20  |
| 37  | RR    | 101/101 (100%) | 85 (84%)  | 16 (16%) | 2           | 14  |
| 37  | YR    | 101/101 (100%) | 85 (84%)  | 16 (16%) | 2           | 14  |
| 38  | RS    | 87/88 (99%)    | 73 (84%)  | 14 (16%) | 2           | 14  |
| 38  | YS    | 87/88 (99%)    | 73 (84%)  | 14 (16%) | 2           | 14  |
| 39  | RT    | 120/127 (94%)  | 99 (82%)  | 21 (18%) | 2           | 11  |
| 39  | YT    | 120/127 (94%)  | 100 (83%) | 20 (17%) | 2           | 13  |
| 40  | RU    | 93/94 (99%)    | 81 (87%)  | 12 (13%) | 4           | 21  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 40  | YU    | 93/94 (99%)   | 81 (87%)  | 12 (13%) | 4           | 21 |
| 41  | RV    | 82/82 (100%)  | 67 (82%)  | 15 (18%) | 2           | 10 |
| 41  | YV    | 82/82 (100%)  | 66 (80%)  | 16 (20%) | 1           | 8  |
| 42  | RW    | 92/92 (100%)  | 76 (83%)  | 16 (17%) | 2           | 11 |
| 42  | YW    | 92/92 (100%)  | 76 (83%)  | 16 (17%) | 2           | 11 |
| 43  | RX    | 74/78 (95%)   | 61 (82%)  | 13 (18%) | 2           | 11 |
| 43  | YX    | 74/78 (95%)   | 61 (82%)  | 13 (18%) | 2           | 11 |
| 44  | RY    | 85/91 (93%)   | 67 (79%)  | 18 (21%) | 1           | 6  |
| 44  | YY    | 85/91 (93%)   | 66 (78%)  | 19 (22%) | 1           | 5  |
| 45  | RZ    | 162/179 (90%) | 136 (84%) | 26 (16%) | 2           | 14 |
| 45  | YZ    | 162/179 (90%) | 137 (85%) | 25 (15%) | 2           | 16 |
| 46  | R0    | 65/67 (97%)   | 60 (92%)  | 5 (8%)   | 12          | 37 |
| 46  | Y0    | 65/67 (97%)   | 59 (91%)  | 6 (9%)   | 8           | 32 |
| 47  | R1    | 82/83 (99%)   | 70 (85%)  | 12 (15%) | 3           | 17 |
| 47  | Y1    | 82/83 (99%)   | 70 (85%)  | 12 (15%) | 3           | 17 |
| 48  | R2    | 64/67 (96%)   | 56 (88%)  | 8 (12%)  | 4           | 22 |
| 48  | Y2    | 64/67 (96%)   | 56 (88%)  | 8 (12%)  | 4           | 22 |
| 49  | R3    | 51/52 (98%)   | 41 (80%)  | 10 (20%) | 1           | 8  |
| 49  | Y3    | 51/52 (98%)   | 41 (80%)  | 10 (20%) | 1           | 8  |
| 50  | R4    | 63/63 (100%)  | 46 (73%)  | 17 (27%) | 0           | 3  |
| 50  | Y4    | 63/63 (100%)  | 46 (73%)  | 17 (27%) | 0           | 3  |
| 51  | R5    | 51/52 (98%)   | 40 (78%)  | 11 (22%) | 1           | 6  |
| 51  | Y5    | 51/52 (98%)   | 40 (78%)  | 11 (22%) | 1           | 6  |
| 52  | R6    | 48/52 (92%)   | 36 (75%)  | 12 (25%) | 0           | 4  |
| 52  | Y6    | 48/52 (92%)   | 36 (75%)  | 12 (25%) | 0           | 4  |
| 53  | R7    | 42/42 (100%)  | 38 (90%)  | 4 (10%)  | 8           | 31 |
| 53  | Y7    | 42/42 (100%)  | 38 (90%)  | 4 (10%)  | 8           | 31 |
| 54  | R8    | 54/55 (98%)   | 41 (76%)  | 13 (24%) | 1           | 4  |
| 54  | Y8    | 54/55 (98%)   | 40 (74%)  | 14 (26%) | 0           | 3  |
| 55  | R9    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 18          | 45 |
| 55  | Y9    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 18          | 45 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |
|-----|-------|------------------|------------|------------|-------------|
| All | All   | 9702/10066 (96%) | 8223 (85%) | 1479 (15%) | 3 16        |

All (1479) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 5   | ILE  |
| 2   | QB    | 8   | LYS  |
| 2   | QB    | 20  | GLU  |
| 2   | QB    | 23  | ARG  |
| 2   | QB    | 24  | TRP  |
| 2   | QB    | 36  | ARG  |
| 2   | QB    | 63  | MET  |
| 2   | QB    | 67  | THR  |
| 2   | QB    | 73  | THR  |
| 2   | QB    | 75  | LYS  |
| 2   | QB    | 90  | MET  |
| 2   | QB    | 92  | TYR  |
| 2   | QB    | 94  | ASN  |
| 2   | QB    | 121 | LEU  |
| 2   | QB    | 155 | LEU  |
| 2   | QB    | 163 | PHE  |
| 2   | QB    | 165 | VAL  |
| 2   | QB    | 168 | THR  |
| 2   | QB    | 172 | ILE  |
| 2   | QB    | 174 | VAL  |
| 2   | QB    | 178 | ARG  |
| 2   | QB    | 215 | LEU  |
| 2   | QB    | 222 | ILE  |
| 3   | QC    | 3   | ASN  |
| 3   | QC    | 5   | ILE  |
| 3   | QC    | 12  | LEU  |
| 3   | QC    | 16  | ARG  |
| 3   | QC    | 21  | ARG  |
| 3   | QC    | 27  | LYS  |
| 3   | QC    | 45  | LYS  |
| 3   | QC    | 56  | ASP  |
| 3   | QC    | 69  | HIS  |
| 3   | QC    | 82  | GLU  |
| 3   | QC    | 127 | ARG  |
| 3   | QC    | 131 | ARG  |
| 3   | QC    | 154 | SER  |
| 3   | QC    | 192 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | QC    | 193 | TYR  |
| 3   | QC    | 196 | LEU  |
| 3   | QC    | 198 | VAL  |
| 4   | QD    | 3   | ARG  |
| 4   | QD    | 7   | PRO  |
| 4   | QD    | 9   | CYS  |
| 4   | QD    | 12  | CYS  |
| 4   | QD    | 13  | ARG  |
| 4   | QD    | 14  | ARG  |
| 4   | QD    | 30  | LYS  |
| 4   | QD    | 31  | CYS  |
| 4   | QD    | 33  | MET  |
| 4   | QD    | 50  | ARG  |
| 4   | QD    | 53  | ASP  |
| 4   | QD    | 58  | LEU  |
| 4   | QD    | 73  | ARG  |
| 4   | QD    | 79  | PHE  |
| 4   | QD    | 86  | LYS  |
| 4   | QD    | 94  | LEU  |
| 4   | QD    | 96  | LEU  |
| 4   | QD    | 112 | VAL  |
| 4   | QD    | 114 | ARG  |
| 4   | QD    | 127 | THR  |
| 4   | QD    | 131 | ARG  |
| 4   | QD    | 146 | ILE  |
| 4   | QD    | 181 | MET  |
| 4   | QD    | 196 | LEU  |
| 5   | QE    | 10  | MET  |
| 5   | QE    | 13  | ILE  |
| 5   | QE    | 16  | THR  |
| 5   | QE    | 31  | LEU  |
| 5   | QE    | 51  | VAL  |
| 5   | QE    | 53  | LEU  |
| 5   | QE    | 79  | GLU  |
| 5   | QE    | 101 | ILE  |
| 5   | QE    | 112 | LEU  |
| 5   | QE    | 140 | ARG  |
| 5   | QE    | 153 | LYS  |
| 6   | QF    | 17  | SER  |
| 6   | QF    | 21  | LEU  |
| 6   | QF    | 27  | GLN  |
| 6   | QF    | 36  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | QF    | 45  | LEU  |
| 6   | QF    | 55  | ASP  |
| 6   | QF    | 63  | TYR  |
| 6   | QF    | 74  | ASP  |
| 6   | QF    | 77  | ARG  |
| 6   | QF    | 92  | LYS  |
| 6   | QF    | 94  | GLN  |
| 6   | QF    | 97  | PHE  |
| 6   | QF    | 100 | ASN  |
| 7   | QG    | 8   | GLU  |
| 7   | QG    | 12  | LEU  |
| 7   | QG    | 30  | ILE  |
| 7   | QG    | 38  | LEU  |
| 7   | QG    | 84  | ASN  |
| 7   | QG    | 98  | SER  |
| 7   | QG    | 104 | LEU  |
| 7   | QG    | 111 | ARG  |
| 7   | QG    | 122 | HIS  |
| 7   | QG    | 124 | LEU  |
| 7   | QG    | 126 | ASP  |
| 7   | QG    | 137 | LYS  |
| 7   | QG    | 148 | ASN  |
| 7   | QG    | 155 | ARG  |
| 8   | QH    | 1   | MET  |
| 8   | QH    | 6   | ILE  |
| 8   | QH    | 10  | LEU  |
| 8   | QH    | 26  | VAL  |
| 8   | QH    | 27  | PRO  |
| 8   | QH    | 41  | ARG  |
| 8   | QH    | 52  | ASP  |
| 8   | QH    | 63  | LEU  |
| 8   | QH    | 83  | ILE  |
| 8   | QH    | 99  | GLU  |
| 8   | QH    | 119 | LEU  |
| 8   | QH    | 121 | ASP  |
| 8   | QH    | 129 | VAL  |
| 8   | QH    | 137 | VAL  |
| 9   | QI    | 7   | THR  |
| 9   | QI    | 9   | ARG  |
| 9   | QI    | 47  | LEU  |
| 9   | QI    | 48  | GLU  |
| 9   | QI    | 65  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | QI    | 83  | ARG  |
| 9   | QI    | 85  | LEU  |
| 9   | QI    | 95  | LYS  |
| 9   | QI    | 104 | ARG  |
| 9   | QI    | 113 | LYS  |
| 9   | QI    | 114 | TYR  |
| 9   | QI    | 118 | LYS  |
| 9   | QI    | 128 | ARG  |
| 10  | QJ    | 47  | PHE  |
| 10  | QJ    | 49  | VAL  |
| 10  | QJ    | 57  | LYS  |
| 10  | QJ    | 62  | HIS  |
| 10  | QJ    | 74  | ILE  |
| 10  | QJ    | 80  | LYS  |
| 10  | QJ    | 84  | GLN  |
| 10  | QJ    | 96  | ILE  |
| 10  | QJ    | 98  | ILE  |
| 11  | QK    | 25  | TYR  |
| 11  | QK    | 26  | ASN  |
| 11  | QK    | 32  | ILE  |
| 11  | QK    | 63  | LEU  |
| 11  | QK    | 75  | TYR  |
| 11  | QK    | 92  | GLU  |
| 11  | QK    | 109 | VAL  |
| 11  | QK    | 114 | VAL  |
| 11  | QK    | 125 | PHE  |
| 12  | QL    | 17  | LYS  |
| 12  | QL    | 20  | LYS  |
| 12  | QL    | 24  | VAL  |
| 12  | QL    | 27  | LEU  |
| 12  | QL    | 41  | ARG  |
| 12  | QL    | 57  | LYS  |
| 12  | QL    | 62  | SER  |
| 12  | QL    | 70  | ILE  |
| 12  | QL    | 73  | GLU  |
| 12  | QL    | 81  | SER  |
| 12  | QL    | 101 | VAL  |
| 12  | QL    | 104 | VAL  |
| 12  | QL    | 110 | VAL  |
| 12  | QL    | 112 | ASP  |
| 12  | QL    | 116 | SER  |
| 12  | QL    | 120 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | QL    | 126 | LYS  |
| 13  | QM    | 3   | ARG  |
| 13  | QM    | 8   | GLU  |
| 13  | QM    | 13  | LYS  |
| 13  | QM    | 35  | GLU  |
| 13  | QM    | 47  | ASP  |
| 13  | QM    | 56  | LEU  |
| 13  | QM    | 57  | ARG  |
| 13  | QM    | 66  | LEU  |
| 13  | QM    | 70  | LEU  |
| 13  | QM    | 88  | ARG  |
| 13  | QM    | 101 | GLN  |
| 13  | QM    | 115 | LYS  |
| 13  | QM    | 116 | THR  |
| 13  | QM    | 122 | LYS  |
| 14  | QN    | 3   | ARG  |
| 14  | QN    | 12  | ARG  |
| 14  | QN    | 14  | PRO  |
| 14  | QN    | 16  | PHE  |
| 14  | QN    | 26  | ARG  |
| 14  | QN    | 29  | ARG  |
| 14  | QN    | 41  | ARG  |
| 14  | QN    | 43  | CYS  |
| 14  | QN    | 44  | LEU  |
| 15  | QO    | 3   | ILE  |
| 15  | QO    | 6   | GLU  |
| 15  | QO    | 8   | LYS  |
| 15  | QO    | 26  | GLU  |
| 15  | QO    | 39  | LEU  |
| 15  | QO    | 62  | GLN  |
| 15  | QO    | 65  | ARG  |
| 15  | QO    | 67  | LEU  |
| 15  | QO    | 82  | ILE  |
| 16  | QP    | 11  | SER  |
| 16  | QP    | 26  | ARG  |
| 16  | QP    | 28  | ARG  |
| 16  | QP    | 59  | TRP  |
| 16  | QP    | 62  | VAL  |
| 16  | QP    | 69  | THR  |
| 16  | QP    | 71  | ARG  |
| 16  | QP    | 82  | GLN  |
| 17  | QQ    | 9   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | QQ    | 12  | SER  |
| 17  | QQ    | 38  | ARG  |
| 17  | QQ    | 48  | GLU  |
| 17  | QQ    | 52  | LYS  |
| 17  | QQ    | 59  | ILE  |
| 17  | QQ    | 65  | ILE  |
| 17  | QQ    | 68  | ARG  |
| 17  | QQ    | 74  | LEU  |
| 18  | QR    | 26  | LEU  |
| 18  | QR    | 29  | PHE  |
| 18  | QR    | 32  | ARG  |
| 18  | QR    | 36  | ASN  |
| 18  | QR    | 46  | GLU  |
| 18  | QR    | 54  | ARG  |
| 18  | QR    | 55  | ARG  |
| 18  | QR    | 69  | THR  |
| 18  | QR    | 83  | GLU  |
| 18  | QR    | 86  | VAL  |
| 19  | QS    | 5   | LEU  |
| 19  | QS    | 10  | PHE  |
| 19  | QS    | 12  | ASP  |
| 19  | QS    | 15  | LEU  |
| 19  | QS    | 29  | ARG  |
| 19  | QS    | 30  | LEU  |
| 19  | QS    | 41  | VAL  |
| 19  | QS    | 63  | THR  |
| 19  | QS    | 65  | ASN  |
| 19  | QS    | 81  | ARG  |
| 19  | QS    | 83  | HIS  |
| 20  | QT    | 10  | LEU  |
| 20  | QT    | 24  | LEU  |
| 20  | QT    | 26  | ASN  |
| 20  | QT    | 41  | ILE  |
| 20  | QT    | 73  | HIS  |
| 20  | QT    | 75  | ASN  |
| 20  | QT    | 93  | GLU  |
| 27  | RD    | 10  | THR  |
| 27  | RD    | 17  | THR  |
| 27  | RD    | 26  | LYS  |
| 27  | RD    | 28  | GLU  |
| 27  | RD    | 33  | LEU  |
| 27  | RD    | 43  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | RD    | 44  | ASN  |
| 27  | RD    | 52  | ARG  |
| 27  | RD    | 61  | LEU  |
| 27  | RD    | 65  | ILE  |
| 27  | RD    | 73  | VAL  |
| 27  | RD    | 94  | LEU  |
| 27  | RD    | 98  | VAL  |
| 27  | RD    | 105 | ILE  |
| 27  | RD    | 106 | ILE  |
| 27  | RD    | 131 | LEU  |
| 27  | RD    | 134 | ARG  |
| 27  | RD    | 135 | PHE  |
| 27  | RD    | 147 | LEU  |
| 27  | RD    | 155 | LEU  |
| 27  | RD    | 157 | ARG  |
| 27  | RD    | 166 | GLN  |
| 27  | RD    | 173 | VAL  |
| 27  | RD    | 177 | LEU  |
| 27  | RD    | 183 | ARG  |
| 27  | RD    | 192 | THR  |
| 27  | RD    | 198 | ASN  |
| 27  | RD    | 200 | ASP  |
| 27  | RD    | 215 | LEU  |
| 27  | RD    | 217 | ARG  |
| 27  | RD    | 218 | ARG  |
| 27  | RD    | 221 | VAL  |
| 27  | RD    | 226 | MET  |
| 27  | RD    | 230 | ASP  |
| 27  | RD    | 233 | HIS  |
| 27  | RD    | 237 | GLU  |
| 27  | RD    | 257 | LEU  |
| 27  | RD    | 259 | THR  |
| 27  | RD    | 261 | LYS  |
| 27  | RD    | 271 | ILE  |
| 28  | RE    | 2   | LYS  |
| 28  | RE    | 4   | ILE  |
| 28  | RE    | 5   | LEU  |
| 28  | RE    | 13  | ARG  |
| 28  | RE    | 14  | ILE  |
| 28  | RE    | 17  | ASP  |
| 28  | RE    | 21  | VAL  |
| 28  | RE    | 25  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | RE    | 26  | ILE  |
| 28  | RE    | 27  | LEU  |
| 28  | RE    | 33  | VAL  |
| 28  | RE    | 36  | ARG  |
| 28  | RE    | 38  | THR  |
| 28  | RE    | 41  | LYS  |
| 28  | RE    | 45  | THR  |
| 28  | RE    | 48  | GLN  |
| 28  | RE    | 49  | LEU  |
| 28  | RE    | 54  | GLN  |
| 28  | RE    | 59  | VAL  |
| 28  | RE    | 61  | ARG  |
| 28  | RE    | 62  | PRO  |
| 28  | RE    | 66  | HIS  |
| 28  | RE    | 73  | GLU  |
| 28  | RE    | 75  | VAL  |
| 28  | RE    | 77  | ILE  |
| 28  | RE    | 78  | LEU  |
| 28  | RE    | 79  | ARG  |
| 28  | RE    | 80  | GLU  |
| 28  | RE    | 93  | VAL  |
| 28  | RE    | 117 | MET  |
| 28  | RE    | 119 | ARG  |
| 28  | RE    | 143 | ASN  |
| 28  | RE    | 146 | THR  |
| 28  | RE    | 154 | LYS  |
| 28  | RE    | 167 | VAL  |
| 28  | RE    | 179 | GLU  |
| 28  | RE    | 184 | VAL  |
| 28  | RE    | 196 | VAL  |
| 28  | RE    | 200 | GLU  |
| 28  | RE    | 203 | LYS  |
| 29  | RF    | 7   | TYR  |
| 29  | RF    | 9   | ILE  |
| 29  | RF    | 25  | PRO  |
| 29  | RF    | 32  | LEU  |
| 29  | RF    | 33  | LEU  |
| 29  | RF    | 45  | ARG  |
| 29  | RF    | 46  | ARG  |
| 29  | RF    | 65  | TRP  |
| 29  | RF    | 66  | PRO  |
| 29  | RF    | 67  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | RF    | 70  | THR  |
| 29  | RF    | 82  | ILE  |
| 29  | RF    | 106 | ARG  |
| 29  | RF    | 108 | LYS  |
| 29  | RF    | 124 | LEU  |
| 29  | RF    | 127 | GLU  |
| 29  | RF    | 145 | GLU  |
| 29  | RF    | 161 | GLU  |
| 29  | RF    | 164 | ARG  |
| 29  | RF    | 179 | GLU  |
| 29  | RF    | 181 | LEU  |
| 29  | RF    | 183 | VAL  |
| 29  | RF    | 206 | ILE  |
| 30  | RG    | 4   | ASP  |
| 30  | RG    | 22  | ARG  |
| 30  | RG    | 26  | GLN  |
| 30  | RG    | 34  | LEU  |
| 30  | RG    | 40  | ASN  |
| 30  | RG    | 43  | LEU  |
| 30  | RG    | 45  | GLU  |
| 30  | RG    | 63  | ILE  |
| 30  | RG    | 67  | LYS  |
| 30  | RG    | 71  | THR  |
| 30  | RG    | 88  | ILE  |
| 30  | RG    | 94  | LEU  |
| 30  | RG    | 96  | ARG  |
| 30  | RG    | 103 | LEU  |
| 30  | RG    | 115 | ARG  |
| 30  | RG    | 118 | ARG  |
| 30  | RG    | 135 | LEU  |
| 30  | RG    | 147 | ASP  |
| 30  | RG    | 155 | MET  |
| 30  | RG    | 156 | ASP  |
| 30  | RG    | 159 | VAL  |
| 30  | RG    | 174 | GLU  |
| 31  | RH    | 3   | ARG  |
| 31  | RH    | 4   | ILE  |
| 31  | RH    | 9   | ILE  |
| 31  | RH    | 10  | PRO  |
| 31  | RH    | 11  | VAL  |
| 31  | RH    | 16  | SER  |
| 31  | RH    | 27  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | RH    | 32  | GLU  |
| 31  | RH    | 37  | VAL  |
| 31  | RH    | 41  | MET  |
| 31  | RH    | 43  | VAL  |
| 31  | RH    | 44  | VAL  |
| 31  | RH    | 47  | GLU  |
| 31  | RH    | 59  | ARG  |
| 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    | 124 | GLU  |
| 31  | RH    | 132 | ARG  |
| 31  | RH    | 136 | ILE  |
| 31  | RH    | 139 | GLN  |
| 31  | RH    | 143 | GLN  |
| 31  | RH    | 144 | VAL  |
| 31  | RH    | 152 | ARG  |
| 31  | RH    | 153 | LYS  |
| 31  | RH    | 154 | PRO  |
| 31  | RH    | 155 | SER  |
| 31  | RH    | 169 | VAL  |
| 32  | RI    | 2   | LYS  |
| 32  | RI    | 10  | GLU  |
| 32  | RI    | 27  | ARG  |
| 32  | RI    | 31  | LEU  |
| 32  | RI    | 35  | LEU  |
| 32  | RI    | 38  | LEU  |
| 32  | RI    | 51  | ILE  |
| 32  | RI    | 56  | LYS  |
| 32  | RI    | 57  | ARG  |
| 32  | RI    | 67  | ARG  |
| 32  | RI    | 70  | GLU  |
| 32  | RI    | 73  | GLU  |
| 32  | RI    | 85  | GLU  |
| 32  | RI    | 86  | THR  |
| 32  | RI    | 88  | ILE  |
| 32  | RI    | 92  | VAL  |
| 32  | RI    | 93  | THR  |
| 32  | RI    | 96  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | RI    | 101 | LEU  |
| 32  | RI    | 118 | LYS  |
| 32  | RI    | 128 | LEU  |
| 32  | RI    | 135 | GLU  |
| 32  | RI    | 136 | VAL  |
| 32  | RI    | 138 | ILE  |
| 32  | RI    | 139 | GLN  |
| 32  | RI    | 142 | VAL  |
| 32  | RI    | 145 | VAL  |
| 33  | RN    | 2   | LYS  |
| 33  | RN    | 7   | LYS  |
| 33  | RN    | 43  | THR  |
| 33  | RN    | 48  | MET  |
| 33  | RN    | 60  | ILE  |
| 33  | RN    | 61  | ARG  |
| 33  | RN    | 65  | LYS  |
| 33  | RN    | 73  | THR  |
| 33  | RN    | 78  | TYR  |
| 33  | RN    | 90  | MET  |
| 33  | RN    | 93  | THR  |
| 33  | RN    | 94  | HIS  |
| 33  | RN    | 98  | VAL  |
| 33  | RN    | 101 | HIS  |
| 33  | RN    | 109 | LYS  |
| 33  | RN    | 112 | LEU  |
| 33  | RN    | 120 | LEU  |
| 33  | RN    | 127 | ASP  |
| 33  | RN    | 131 | GLN  |
| 33  | RN    | 136 | GLU  |
| 34  | RO    | 8   | LEU  |
| 34  | RO    | 9   | GLU  |
| 34  | RO    | 19  | ILE  |
| 34  | RO    | 23  | ARG  |
| 34  | RO    | 39  | ILE  |
| 34  | RO    | 49  | ARG  |
| 34  | RO    | 52  | VAL  |
| 34  | RO    | 53  | LYS  |
| 34  | RO    | 63  | VAL  |
| 34  | RO    | 65  | THR  |
| 34  | RO    | 91  | LEU  |
| 35  | RP    | 5   | ASP  |
| 35  | RP    | 9   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | RP    | 10  | PRO  |
| 35  | RP    | 14  | LYS  |
| 35  | RP    | 16  | ARG  |
| 35  | RP    | 21  | ARG  |
| 35  | RP    | 27  | HIS  |
| 35  | RP    | 29  | LYS  |
| 35  | RP    | 30  | THR  |
| 35  | RP    | 32  | THR  |
| 35  | RP    | 33  | ARG  |
| 35  | RP    | 36  | LYS  |
| 35  | RP    | 50  | ARG  |
| 35  | RP    | 55  | ARG  |
| 35  | RP    | 61  | ARG  |
| 35  | RP    | 62  | LEU  |
| 35  | RP    | 64  | LYS  |
| 35  | RP    | 65  | ARG  |
| 35  | RP    | 75  | ILE  |
| 35  | RP    | 81  | GLN  |
| 35  | RP    | 88  | LEU  |
| 35  | RP    | 91  | PHE  |
| 35  | RP    | 99  | LEU  |
| 35  | RP    | 100 | LEU  |
| 35  | RP    | 105 | LEU  |
| 35  | RP    | 144 | GLU  |
| 35  | RP    | 146 | VAL  |
| 35  | RP    | 149 | GLU  |
| 36  | RQ    | 2   | LEU  |
| 36  | RQ    | 25  | ASP  |
| 36  | RQ    | 26  | TYR  |
| 36  | RQ    | 27  | VAL  |
| 36  | RQ    | 54  | MET  |
| 36  | RQ    | 55  | VAL  |
| 36  | RQ    | 58  | PHE  |
| 36  | RQ    | 60  | ARG  |
| 36  | RQ    | 79  | LEU  |
| 36  | RQ    | 83  | MET  |
| 36  | RQ    | 89  | ASN  |
| 36  | RQ    | 90  | VAL  |
| 36  | RQ    | 91  | GLU  |
| 36  | RQ    | 112 | GLU  |
| 36  | RQ    | 139 | GLU  |
| 37  | RR    | 14  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | RR    | 37  | THR  |
| 37  | RR    | 44  | LEU  |
| 37  | RR    | 51  | LEU  |
| 37  | RR    | 66  | VAL  |
| 37  | RR    | 67  | LEU  |
| 37  | RR    | 71  | GLN  |
| 37  | RR    | 75  | LEU  |
| 37  | RR    | 76  | VAL  |
| 37  | RR    | 81  | ASP  |
| 37  | RR    | 95  | THR  |
| 37  | RR    | 100 | LEU  |
| 37  | RR    | 104 | ARG  |
| 37  | RR    | 105 | ARG  |
| 37  | RR    | 107 | ASP  |
| 37  | RR    | 113 | LEU  |
| 38  | RS    | 4   | LEU  |
| 38  | RS    | 12  | PHE  |
| 38  | RS    | 17  | ARG  |
| 38  | RS    | 18  | ILE  |
| 38  | RS    | 20  | ARG  |
| 38  | RS    | 44  | LYS  |
| 38  | RS    | 56  | LEU  |
| 38  | RS    | 57  | LYS  |
| 38  | RS    | 73  | LEU  |
| 38  | RS    | 89  | ARG  |
| 38  | RS    | 101 | LEU  |
| 38  | RS    | 103 | GLU  |
| 38  | RS    | 106 | ARG  |
| 38  | RS    | 111 | GLU  |
| 39  | RT    | 2   | ASN  |
| 39  | RT    | 14  | TYR  |
| 39  | RT    | 22  | PHE  |
| 39  | RT    | 23  | ARG  |
| 39  | RT    | 27  | THR  |
| 39  | RT    | 42  | ILE  |
| 39  | RT    | 48  | ILE  |
| 39  | RT    | 50  | ILE  |
| 39  | RT    | 58  | ASN  |
| 39  | RT    | 65  | LYS  |
| 39  | RT    | 73  | GLU  |
| 39  | RT    | 78  | LEU  |
| 39  | RT    | 86  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | RT    | 87  | ASP  |
| 39  | RT    | 100 | TYR  |
| 39  | RT    | 104 | ASN  |
| 39  | RT    | 107 | ASP  |
| 39  | RT    | 111 | ARG  |
| 39  | RT    | 112 | ARG  |
| 39  | RT    | 128 | GLU  |
| 39  | RT    | 134 | GLU  |
| 40  | RU    | 5   | LYS  |
| 40  | RU    | 9   | VAL  |
| 40  | RU    | 31  | SER  |
| 40  | RU    | 52  | ARG  |
| 40  | RU    | 60  | LEU  |
| 40  | RU    | 64  | ARG  |
| 40  | RU    | 79  | PHE  |
| 40  | RU    | 88  | ILE  |
| 40  | RU    | 92  | ARG  |
| 40  | RU    | 98  | LEU  |
| 40  | RU    | 108 | GLU  |
| 40  | RU    | 117 | GLN  |
| 41  | RV    | 14  | VAL  |
| 41  | RV    | 18  | LEU  |
| 41  | RV    | 24  | LYS  |
| 41  | RV    | 35  | LEU  |
| 41  | RV    | 38  | LEU  |
| 41  | RV    | 39  | LEU  |
| 41  | RV    | 40  | LEU  |
| 41  | RV    | 47  | VAL  |
| 41  | RV    | 57  | VAL  |
| 41  | RV    | 61  | VAL  |
| 41  | RV    | 66  | ARG  |
| 41  | RV    | 70  | ILE  |
| 41  | RV    | 75  | PHE  |
| 41  | RV    | 91  | TYR  |
| 41  | RV    | 99  | ILE  |
| 42  | RW    | 11  | ARG  |
| 42  | RW    | 14  | PRO  |
| 42  | RW    | 16  | LYS  |
| 42  | RW    | 19  | LEU  |
| 42  | RW    | 20  | VAL  |
| 42  | RW    | 23  | LEU  |
| 42  | RW    | 63  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | RW    | 67  | ASP  |
| 42  | RW    | 69  | LEU  |
| 42  | RW    | 70  | TYR  |
| 42  | RW    | 87  | PRO  |
| 42  | RW    | 88  | ARG  |
| 42  | RW    | 92  | ARG  |
| 42  | RW    | 95  | ILE  |
| 42  | RW    | 107 | LEU  |
| 42  | RW    | 109 | GLU  |
| 43  | RX    | 3   | THR  |
| 43  | RX    | 15  | GLU  |
| 43  | RX    | 27  | THR  |
| 43  | RX    | 30  | VAL  |
| 43  | RX    | 49  | VAL  |
| 43  | RX    | 57  | LEU  |
| 43  | RX    | 65  | ARG  |
| 43  | RX    | 70  | LEU  |
| 43  | RX    | 72  | LYS  |
| 43  | RX    | 76  | ARG  |
| 43  | RX    | 80  | ILE  |
| 43  | RX    | 81  | VAL  |
| 43  | RX    | 88  | LYS  |
| 44  | RY    | 7   | VAL  |
| 44  | RY    | 26  | LYS  |
| 44  | RY    | 27  | VAL  |
| 44  | RY    | 42  | VAL  |
| 44  | RY    | 45  | VAL  |
| 44  | RY    | 57  | GLN  |
| 44  | RY    | 61  | ILE  |
| 44  | RY    | 64  | GLU  |
| 44  | RY    | 72  | VAL  |
| 44  | RY    | 75  | ILE  |
| 44  | RY    | 77  | PRO  |
| 44  | RY    | 79  | CYS  |
| 44  | RY    | 87  | LYS  |
| 44  | RY    | 88  | LYS  |
| 44  | RY    | 89  | PHE  |
| 44  | RY    | 90  | LEU  |
| 44  | RY    | 95  | LYS  |
| 44  | RY    | 97  | ARG  |
| 45  | RZ    | 2   | GLU  |
| 45  | RZ    | 19  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | RZ    | 20  | ARG  |
| 45  | RZ    | 35  | ARG  |
| 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    | 94  | GLU  |
| 45  | RZ    | 111 | VAL  |
| 45  | RZ    | 119 | GLU  |
| 45  | RZ    | 121 | HIS  |
| 45  | RZ    | 128 | VAL  |
| 45  | RZ    | 141 | VAL  |
| 45  | RZ    | 145 | GLU  |
| 45  | RZ    | 148 | ASP  |
| 45  | RZ    | 150 | LEU  |
| 45  | RZ    | 163 | LEU  |
| 45  | RZ    | 166 | SER  |
| 45  | RZ    | 168 | GLU  |
| 45  | RZ    | 174 | VAL  |
| 45  | RZ    | 182 | LYS  |
| 45  | RZ    | 183 | LEU  |
| 46  | R0    | 7   | LEU  |
| 46  | R0    | 11  | ARG  |
| 46  | R0    | 36  | ILE  |
| 46  | R0    | 66  | VAL  |
| 46  | R0    | 74  | ARG  |
| 47  | R1    | 2   | SER  |
| 47  | R1    | 11  | ARG  |
| 47  | R1    | 30  | VAL  |
| 47  | R1    | 41  | ARG  |
| 47  | R1    | 56  | GLN  |
| 47  | R1    | 75  | GLU  |
| 47  | R1    | 80  | LEU  |
| 47  | R1    | 81  | LYS  |
| 47  | R1    | 83  | GLU  |
| 47  | R1    | 87  | PRO  |
| 47  | R1    | 91  | LYS  |
| 47  | R1    | 97  | LEU  |
| 48  | R2    | 7   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | R2    | 9   | GLN  |
| 48  | R2    | 16  | LEU  |
| 48  | R2    | 24  | LEU  |
| 48  | R2    | 47  | ASN  |
| 48  | R2    | 53  | LEU  |
| 48  | R2    | 62  | THR  |
| 48  | R2    | 64  | LEU  |
| 49  | R3    | 4   | LEU  |
| 49  | R3    | 8   | LEU  |
| 49  | R3    | 9   | VAL  |
| 49  | R3    | 10  | LYS  |
| 49  | R3    | 30  | ARG  |
| 49  | R3    | 31  | LEU  |
| 49  | R3    | 32  | GLN  |
| 49  | R3    | 37  | LEU  |
| 49  | R3    | 40  | THR  |
| 49  | R3    | 44  | ARG  |
| 50  | R4    | 6   | HIS  |
| 50  | R4    | 15  | ILE  |
| 50  | R4    | 18  | CYS  |
| 50  | R4    | 21  | VAL  |
| 50  | R4    | 23  | GLU  |
| 50  | R4    | 39  | CYS  |
| 50  | R4    | 42  | PHE  |
| 50  | R4    | 49  | PHE  |
| 50  | R4    | 50  | VAL  |
| 50  | R4    | 53  | GLU  |
| 50  | R4    | 57  | GLU  |
| 50  | R4    | 61  | ARG  |
| 50  | R4    | 62  | ARG  |
| 50  | R4    | 63  | TYR  |
| 50  | R4    | 68  | ARG  |
| 50  | R4    | 69  | LYS  |
| 50  | R4    | 71  | ARG  |
| 51  | R5    | 3   | LYS  |
| 51  | R5    | 4   | HIS  |
| 51  | R5    | 6   | VAL  |
| 51  | R5    | 11  | THR  |
| 51  | R5    | 19  | ARG  |
| 51  | R5    | 25  | LEU  |
| 51  | R5    | 36  | CYS  |
| 51  | R5    | 37  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | R5    | 52  | TYR  |
| 51  | R5    | 56  | LYS  |
| 51  | R5    | 58  | LEU  |
| 52  | R6    | 6   | ARG  |
| 52  | R6    | 8   | LYS  |
| 52  | R6    | 10  | LEU  |
| 52  | R6    | 18  | ARG  |
| 52  | R6    | 19  | ARG  |
| 52  | R6    | 27  | LYS  |
| 52  | R6    | 33  | LYS  |
| 52  | R6    | 34  | LEU  |
| 52  | R6    | 37  | ARG  |
| 52  | R6    | 42  | TRP  |
| 52  | R6    | 44  | ARG  |
| 52  | R6    | 53  | LYS  |
| 53  | R7    | 1   | MET  |
| 53  | R7    | 9   | ARG  |
| 53  | R7    | 14  | LYS  |
| 53  | R7    | 43  | THR  |
| 54  | R8    | 16  | ILE  |
| 54  | R8    | 35  | GLN  |
| 54  | R8    | 39  | LYS  |
| 54  | R8    | 43  | GLN  |
| 54  | R8    | 47  | LYS  |
| 54  | R8    | 48  | PHE  |
| 54  | R8    | 49  | VAL  |
| 54  | R8    | 52  | LYS  |
| 54  | R8    | 53  | PRO  |
| 54  | R8    | 59  | LYS  |
| 54  | R8    | 62  | LEU  |
| 54  | R8    | 63  | PRO  |
| 54  | R8    | 65  | GLU  |
| 55  | R9    | 1   | MET  |
| 55  | R9    | 17  | ILE  |
| 2   | XB    | 5   | ILE  |
| 2   | XB    | 8   | LYS  |
| 2   | XB    | 20  | GLU  |
| 2   | XB    | 23  | ARG  |
| 2   | XB    | 24  | TRP  |
| 2   | XB    | 36  | ARG  |
| 2   | XB    | 63  | MET  |
| 2   | XB    | 67  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | XB    | 73  | THR  |
| 2   | XB    | 75  | LYS  |
| 2   | XB    | 90  | MET  |
| 2   | XB    | 92  | TYR  |
| 2   | XB    | 94  | ASN  |
| 2   | XB    | 121 | LEU  |
| 2   | XB    | 155 | LEU  |
| 2   | XB    | 163 | PHE  |
| 2   | XB    | 165 | VAL  |
| 2   | XB    | 168 | THR  |
| 2   | XB    | 172 | ILE  |
| 2   | XB    | 174 | VAL  |
| 2   | XB    | 178 | ARG  |
| 2   | XB    | 196 | LEU  |
| 2   | XB    | 215 | LEU  |
| 2   | XB    | 222 | ILE  |
| 3   | XC    | 3   | ASN  |
| 3   | XC    | 5   | ILE  |
| 3   | XC    | 12  | LEU  |
| 3   | XC    | 16  | ARG  |
| 3   | XC    | 21  | ARG  |
| 3   | XC    | 27  | LYS  |
| 3   | XC    | 45  | LYS  |
| 3   | XC    | 56  | ASP  |
| 3   | XC    | 69  | HIS  |
| 3   | XC    | 82  | GLU  |
| 3   | XC    | 127 | ARG  |
| 3   | XC    | 131 | ARG  |
| 3   | XC    | 154 | SER  |
| 3   | XC    | 192 | THR  |
| 3   | XC    | 193 | TYR  |
| 3   | XC    | 196 | LEU  |
| 3   | XC    | 198 | VAL  |
| 4   | XD    | 3   | ARG  |
| 4   | XD    | 7   | PRO  |
| 4   | XD    | 9   | CYS  |
| 4   | XD    | 30  | LYS  |
| 4   | XD    | 50  | ARG  |
| 4   | XD    | 53  | ASP  |
| 4   | XD    | 58  | LEU  |
| 4   | XD    | 79  | PHE  |
| 4   | XD    | 86  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | XD    | 94  | LEU  |
| 4   | XD    | 96  | LEU  |
| 4   | XD    | 112 | VAL  |
| 4   | XD    | 114 | ARG  |
| 4   | XD    | 127 | THR  |
| 4   | XD    | 131 | ARG  |
| 4   | XD    | 146 | ILE  |
| 4   | XD    | 181 | MET  |
| 4   | XD    | 196 | LEU  |
| 5   | XE    | 10  | MET  |
| 5   | XE    | 13  | ILE  |
| 5   | XE    | 16  | THR  |
| 5   | XE    | 31  | LEU  |
| 5   | XE    | 51  | VAL  |
| 5   | XE    | 53  | LEU  |
| 5   | XE    | 79  | GLU  |
| 5   | XE    | 101 | ILE  |
| 5   | XE    | 112 | LEU  |
| 5   | XE    | 140 | ARG  |
| 5   | XE    | 153 | LYS  |
| 6   | XF    | 17  | SER  |
| 6   | XF    | 21  | LEU  |
| 6   | XF    | 27  | GLN  |
| 6   | XF    | 36  | ARG  |
| 6   | XF    | 45  | LEU  |
| 6   | XF    | 55  | ASP  |
| 6   | XF    | 63  | TYR  |
| 6   | XF    | 74  | ASP  |
| 6   | XF    | 77  | ARG  |
| 6   | XF    | 92  | LYS  |
| 6   | XF    | 94  | GLN  |
| 6   | XF    | 97  | PHE  |
| 6   | XF    | 100 | ASN  |
| 7   | XG    | 8   | GLU  |
| 7   | XG    | 12  | LEU  |
| 7   | XG    | 30  | ILE  |
| 7   | XG    | 38  | LEU  |
| 7   | XG    | 84  | ASN  |
| 7   | XG    | 98  | SER  |
| 7   | XG    | 104 | LEU  |
| 7   | XG    | 111 | ARG  |
| 7   | XG    | 122 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | XG    | 124 | LEU  |
| 7   | XG    | 126 | ASP  |
| 7   | XG    | 137 | LYS  |
| 7   | XG    | 148 | ASN  |
| 7   | XG    | 155 | ARG  |
| 8   | XH    | 1   | MET  |
| 8   | XH    | 10  | LEU  |
| 8   | XH    | 26  | VAL  |
| 8   | XH    | 27  | PRO  |
| 8   | XH    | 41  | ARG  |
| 8   | XH    | 52  | ASP  |
| 8   | XH    | 63  | LEU  |
| 8   | XH    | 83  | ILE  |
| 8   | XH    | 99  | GLU  |
| 8   | XH    | 119 | LEU  |
| 8   | XH    | 121 | ASP  |
| 8   | XH    | 127 | LEU  |
| 8   | XH    | 129 | VAL  |
| 8   | XH    | 137 | VAL  |
| 9   | XI    | 7   | THR  |
| 9   | XI    | 9   | ARG  |
| 9   | XI    | 47  | LEU  |
| 9   | XI    | 48  | GLU  |
| 9   | XI    | 65  | VAL  |
| 9   | XI    | 83  | ARG  |
| 9   | XI    | 85  | LEU  |
| 9   | XI    | 95  | LYS  |
| 9   | XI    | 104 | ARG  |
| 9   | XI    | 113 | LYS  |
| 9   | XI    | 114 | TYR  |
| 9   | XI    | 118 | LYS  |
| 9   | XI    | 128 | ARG  |
| 10  | XJ    | 47  | PHE  |
| 10  | XJ    | 49  | VAL  |
| 10  | XJ    | 57  | LYS  |
| 10  | XJ    | 62  | HIS  |
| 10  | XJ    | 74  | ILE  |
| 10  | XJ    | 80  | LYS  |
| 10  | XJ    | 84  | GLN  |
| 10  | XJ    | 96  | ILE  |
| 10  | XJ    | 98  | ILE  |
| 11  | XK    | 25  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | XK    | 26  | ASN  |
| 11  | XK    | 32  | ILE  |
| 11  | XK    | 63  | LEU  |
| 11  | XK    | 75  | TYR  |
| 11  | XK    | 92  | GLU  |
| 11  | XK    | 109 | VAL  |
| 11  | XK    | 114 | VAL  |
| 11  | XK    | 125 | PHE  |
| 12  | XL    | 17  | LYS  |
| 12  | XL    | 20  | LYS  |
| 12  | XL    | 24  | VAL  |
| 12  | XL    | 27  | LEU  |
| 12  | XL    | 41  | ARG  |
| 12  | XL    | 57  | LYS  |
| 12  | XL    | 60  | LEU  |
| 12  | XL    | 62  | SER  |
| 12  | XL    | 70  | ILE  |
| 12  | XL    | 73  | GLU  |
| 12  | XL    | 81  | SER  |
| 12  | XL    | 101 | VAL  |
| 12  | XL    | 104 | VAL  |
| 12  | XL    | 110 | VAL  |
| 12  | XL    | 112 | ASP  |
| 12  | XL    | 116 | SER  |
| 12  | XL    | 120 | TYR  |
| 12  | XL    | 126 | LYS  |
| 13  | XM    | 3   | ARG  |
| 13  | XM    | 8   | GLU  |
| 13  | XM    | 13  | LYS  |
| 13  | XM    | 35  | GLU  |
| 13  | XM    | 47  | ASP  |
| 13  | XM    | 56  | LEU  |
| 13  | XM    | 57  | ARG  |
| 13  | XM    | 66  | LEU  |
| 13  | XM    | 70  | LEU  |
| 13  | XM    | 88  | ARG  |
| 13  | XM    | 101 | GLN  |
| 13  | XM    | 115 | LYS  |
| 13  | XM    | 116 | THR  |
| 13  | XM    | 122 | LYS  |
| 14  | XN    | 3   | ARG  |
| 14  | XN    | 12  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | XN    | 14  | PRO  |
| 14  | XN    | 16  | PHE  |
| 14  | XN    | 41  | ARG  |
| 15  | XO    | 3   | ILE  |
| 15  | XO    | 6   | GLU  |
| 15  | XO    | 8   | LYS  |
| 15  | XO    | 26  | GLU  |
| 15  | XO    | 39  | LEU  |
| 15  | XO    | 62  | GLN  |
| 15  | XO    | 65  | ARG  |
| 15  | XO    | 67  | LEU  |
| 15  | XO    | 82  | ILE  |
| 16  | XP    | 11  | SER  |
| 16  | XP    | 26  | ARG  |
| 16  | XP    | 28  | ARG  |
| 16  | XP    | 59  | TRP  |
| 16  | XP    | 62  | VAL  |
| 16  | XP    | 69  | THR  |
| 16  | XP    | 71  | ARG  |
| 16  | XP    | 82  | GLN  |
| 17  | XQ    | 9   | VAL  |
| 17  | XQ    | 12  | SER  |
| 17  | XQ    | 38  | ARG  |
| 17  | XQ    | 48  | GLU  |
| 17  | XQ    | 52  | LYS  |
| 17  | XQ    | 59  | ILE  |
| 17  | XQ    | 65  | ILE  |
| 17  | XQ    | 68  | ARG  |
| 17  | XQ    | 74  | LEU  |
| 18  | XR    | 26  | LEU  |
| 18  | XR    | 29  | PHE  |
| 18  | XR    | 32  | ARG  |
| 18  | XR    | 36  | ASN  |
| 18  | XR    | 46  | GLU  |
| 18  | XR    | 54  | ARG  |
| 18  | XR    | 55  | ARG  |
| 18  | XR    | 69  | THR  |
| 18  | XR    | 83  | GLU  |
| 18  | XR    | 86  | VAL  |
| 19  | XS    | 5   | LEU  |
| 19  | XS    | 10  | PHE  |
| 19  | XS    | 12  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | XS    | 15  | LEU  |
| 19  | XS    | 29  | ARG  |
| 19  | XS    | 30  | LEU  |
| 19  | XS    | 41  | VAL  |
| 19  | XS    | 63  | THR  |
| 19  | XS    | 65  | ASN  |
| 19  | XS    | 81  | ARG  |
| 19  | XS    | 83  | HIS  |
| 20  | XT    | 10  | LEU  |
| 20  | XT    | 24  | LEU  |
| 20  | XT    | 26  | ASN  |
| 20  | XT    | 41  | ILE  |
| 20  | XT    | 73  | HIS  |
| 20  | XT    | 75  | ASN  |
| 20  | XT    | 93  | GLU  |
| 27  | YD    | 10  | THR  |
| 27  | YD    | 17  | THR  |
| 27  | YD    | 26  | LYS  |
| 27  | YD    | 28  | GLU  |
| 27  | YD    | 33  | LEU  |
| 27  | YD    | 43  | ARG  |
| 27  | YD    | 44  | ASN  |
| 27  | YD    | 52  | ARG  |
| 27  | YD    | 61  | LEU  |
| 27  | YD    | 65  | ILE  |
| 27  | YD    | 73  | VAL  |
| 27  | YD    | 94  | LEU  |
| 27  | YD    | 98  | VAL  |
| 27  | YD    | 105 | ILE  |
| 27  | YD    | 106 | ILE  |
| 27  | YD    | 131 | LEU  |
| 27  | YD    | 134 | ARG  |
| 27  | YD    | 135 | PHE  |
| 27  | YD    | 147 | LEU  |
| 27  | YD    | 155 | LEU  |
| 27  | YD    | 157 | ARG  |
| 27  | YD    | 166 | GLN  |
| 27  | YD    | 173 | VAL  |
| 27  | YD    | 177 | LEU  |
| 27  | YD    | 183 | ARG  |
| 27  | YD    | 192 | THR  |
| 27  | YD    | 198 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | YD    | 200 | ASP  |
| 27  | YD    | 215 | LEU  |
| 27  | YD    | 217 | ARG  |
| 27  | YD    | 218 | ARG  |
| 27  | YD    | 221 | VAL  |
| 27  | YD    | 226 | MET  |
| 27  | YD    | 230 | ASP  |
| 27  | YD    | 233 | HIS  |
| 27  | YD    | 237 | GLU  |
| 27  | YD    | 257 | LEU  |
| 27  | YD    | 259 | THR  |
| 27  | YD    | 261 | LYS  |
| 27  | YD    | 271 | ILE  |
| 28  | YE    | 2   | LYS  |
| 28  | YE    | 4   | ILE  |
| 28  | YE    | 5   | LEU  |
| 28  | YE    | 13  | ARG  |
| 28  | YE    | 14  | ILE  |
| 28  | YE    | 17  | ASP  |
| 28  | YE    | 21  | VAL  |
| 28  | YE    | 25  | VAL  |
| 28  | YE    | 26  | ILE  |
| 28  | YE    | 27  | LEU  |
| 28  | YE    | 33  | VAL  |
| 28  | YE    | 36  | ARG  |
| 28  | YE    | 38  | THR  |
| 28  | YE    | 41  | LYS  |
| 28  | YE    | 45  | THR  |
| 28  | YE    | 48  | GLN  |
| 28  | YE    | 49  | LEU  |
| 28  | YE    | 54  | GLN  |
| 28  | YE    | 59  | VAL  |
| 28  | YE    | 61  | ARG  |
| 28  | YE    | 62  | PRO  |
| 28  | YE    | 66  | HIS  |
| 28  | YE    | 73  | GLU  |
| 28  | YE    | 75  | VAL  |
| 28  | YE    | 77  | ILE  |
| 28  | YE    | 78  | LEU  |
| 28  | YE    | 79  | ARG  |
| 28  | YE    | 80  | GLU  |
| 28  | YE    | 93  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | YE    | 117 | MET  |
| 28  | YE    | 119 | ARG  |
| 28  | YE    | 143 | ASN  |
| 28  | YE    | 146 | THR  |
| 28  | YE    | 154 | LYS  |
| 28  | YE    | 167 | VAL  |
| 28  | YE    | 179 | GLU  |
| 28  | YE    | 184 | VAL  |
| 28  | YE    | 196 | VAL  |
| 28  | YE    | 200 | GLU  |
| 28  | YE    | 203 | LYS  |
| 29  | YF    | 7   | TYR  |
| 29  | YF    | 9   | ILE  |
| 29  | YF    | 25  | PRO  |
| 29  | YF    | 32  | LEU  |
| 29  | YF    | 33  | LEU  |
| 29  | YF    | 45  | ARG  |
| 29  | YF    | 46  | ARG  |
| 29  | YF    | 65  | TRP  |
| 29  | YF    | 66  | PRO  |
| 29  | YF    | 67  | GLN  |
| 29  | YF    | 70  | THR  |
| 29  | YF    | 82  | ILE  |
| 29  | YF    | 106 | ARG  |
| 29  | YF    | 108 | LYS  |
| 29  | YF    | 124 | LEU  |
| 29  | YF    | 127 | GLU  |
| 29  | YF    | 145 | GLU  |
| 29  | YF    | 161 | GLU  |
| 29  | YF    | 164 | ARG  |
| 29  | YF    | 179 | GLU  |
| 29  | YF    | 181 | LEU  |
| 29  | YF    | 183 | VAL  |
| 29  | YF    | 206 | ILE  |
| 30  | YG    | 4   | ASP  |
| 30  | YG    | 22  | ARG  |
| 30  | YG    | 26  | GLN  |
| 30  | YG    | 34  | LEU  |
| 30  | YG    | 43  | LEU  |
| 30  | YG    | 45  | GLU  |
| 30  | YG    | 63  | ILE  |
| 30  | YG    | 67  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | YG    | 71  | THR  |
| 30  | YG    | 88  | ILE  |
| 30  | YG    | 94  | LEU  |
| 30  | YG    | 96  | ARG  |
| 30  | YG    | 103 | LEU  |
| 30  | YG    | 115 | ARG  |
| 30  | YG    | 118 | ARG  |
| 30  | YG    | 135 | LEU  |
| 30  | YG    | 147 | ASP  |
| 30  | YG    | 155 | MET  |
| 30  | YG    | 156 | ASP  |
| 30  | YG    | 159 | VAL  |
| 30  | YG    | 174 | GLU  |
| 31  | YH    | 3   | ARG  |
| 31  | YH    | 4   | ILE  |
| 31  | YH    | 9   | ILE  |
| 31  | YH    | 10  | PRO  |
| 31  | YH    | 11  | VAL  |
| 31  | YH    | 16  | SER  |
| 31  | YH    | 27  | LYS  |
| 31  | YH    | 32  | GLU  |
| 31  | YH    | 37  | VAL  |
| 31  | YH    | 41  | MET  |
| 31  | YH    | 43  | VAL  |
| 31  | YH    | 44  | VAL  |
| 31  | YH    | 47  | GLU  |
| 31  | YH    | 59  | ARG  |
| 31  | YH    | 64  | LEU  |
| 31  | YH    | 77  | LYS  |
| 31  | YH    | 81  | GLU  |
| 31  | YH    | 88  | LEU  |
| 31  | YH    | 89  | ILE  |
| 31  | YH    | 105 | LEU  |
| 31  | YH    | 124 | GLU  |
| 31  | YH    | 132 | ARG  |
| 31  | YH    | 136 | ILE  |
| 31  | YH    | 139 | GLN  |
| 31  | YH    | 143 | GLN  |
| 31  | YH    | 144 | VAL  |
| 31  | YH    | 152 | ARG  |
| 31  | YH    | 153 | LYS  |
| 31  | YH    | 154 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | YH    | 155 | SER  |
| 31  | YH    | 169 | VAL  |
| 32  | YI    | 1   | MET  |
| 32  | YI    | 2   | LYS  |
| 32  | YI    | 3   | VAL  |
| 32  | YI    | 17  | GLN  |
| 32  | YI    | 35  | LEU  |
| 32  | YI    | 38  | LEU  |
| 32  | YI    | 40  | THR  |
| 32  | YI    | 56  | LYS  |
| 32  | YI    | 67  | ARG  |
| 32  | YI    | 71  | ILE  |
| 32  | YI    | 81  | VAL  |
| 32  | YI    | 85  | GLU  |
| 32  | YI    | 92  | VAL  |
| 32  | YI    | 95  | LYS  |
| 32  | YI    | 101 | LEU  |
| 32  | YI    | 104 | GLN  |
| 32  | YI    | 112 | LYS  |
| 32  | YI    | 118 | LYS  |
| 32  | YI    | 128 | LEU  |
| 32  | YI    | 134 | PRO  |
| 32  | YI    | 135 | GLU  |
| 32  | YI    | 136 | VAL  |
| 32  | YI    | 138 | ILE  |
| 32  | YI    | 139 | GLN  |
| 32  | YI    | 141 | LYS  |
| 32  | YI    | 142 | VAL  |
| 32  | YI    | 145 | VAL  |
| 33  | YN    | 2   | LYS  |
| 33  | YN    | 7   | LYS  |
| 33  | YN    | 43  | THR  |
| 33  | YN    | 48  | MET  |
| 33  | YN    | 60  | ILE  |
| 33  | YN    | 61  | ARG  |
| 33  | YN    | 65  | LYS  |
| 33  | YN    | 73  | THR  |
| 33  | YN    | 78  | TYR  |
| 33  | YN    | 90  | MET  |
| 33  | YN    | 93  | THR  |
| 33  | YN    | 94  | HIS  |
| 33  | YN    | 98  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | YN    | 101 | HIS  |
| 33  | YN    | 109 | LYS  |
| 33  | YN    | 112 | LEU  |
| 33  | YN    | 120 | LEU  |
| 33  | YN    | 127 | ASP  |
| 33  | YN    | 131 | GLN  |
| 33  | YN    | 136 | GLU  |
| 34  | YO    | 8   | LEU  |
| 34  | YO    | 9   | GLU  |
| 34  | YO    | 19  | ILE  |
| 34  | YO    | 23  | ARG  |
| 34  | YO    | 39  | ILE  |
| 34  | YO    | 49  | ARG  |
| 34  | YO    | 52  | VAL  |
| 34  | YO    | 53  | LYS  |
| 34  | YO    | 63  | VAL  |
| 34  | YO    | 65  | THR  |
| 34  | YO    | 91  | LEU  |
| 35  | YP    | 5   | ASP  |
| 35  | YP    | 9   | ASN  |
| 35  | YP    | 10  | PRO  |
| 35  | YP    | 14  | LYS  |
| 35  | YP    | 16  | ARG  |
| 35  | YP    | 21  | ARG  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 29  | LYS  |
| 35  | YP    | 30  | THR  |
| 35  | YP    | 32  | THR  |
| 35  | YP    | 33  | ARG  |
| 35  | YP    | 36  | LYS  |
| 35  | YP    | 50  | ARG  |
| 35  | YP    | 55  | ARG  |
| 35  | YP    | 61  | ARG  |
| 35  | YP    | 62  | LEU  |
| 35  | YP    | 64  | LYS  |
| 35  | YP    | 65  | ARG  |
| 35  | YP    | 75  | ILE  |
| 35  | YP    | 81  | GLN  |
| 35  | YP    | 88  | LEU  |
| 35  | YP    | 91  | PHE  |
| 35  | YP    | 99  | LEU  |
| 35  | YP    | 100 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | YP    | 105 | LEU  |
| 35  | YP    | 144 | GLU  |
| 35  | YP    | 146 | VAL  |
| 35  | YP    | 149 | GLU  |
| 36  | YQ    | 2   | LEU  |
| 36  | YQ    | 25  | ASP  |
| 36  | YQ    | 26  | TYR  |
| 36  | YQ    | 27  | VAL  |
| 36  | YQ    | 54  | MET  |
| 36  | YQ    | 55  | VAL  |
| 36  | YQ    | 59  | ARG  |
| 36  | YQ    | 79  | LEU  |
| 36  | YQ    | 83  | MET  |
| 36  | YQ    | 89  | ASN  |
| 36  | YQ    | 90  | VAL  |
| 36  | YQ    | 91  | GLU  |
| 36  | YQ    | 106 | VAL  |
| 36  | YQ    | 112 | GLU  |
| 36  | YQ    | 139 | GLU  |
| 37  | YR    | 14  | SER  |
| 37  | YR    | 37  | THR  |
| 37  | YR    | 44  | LEU  |
| 37  | YR    | 51  | LEU  |
| 37  | YR    | 66  | VAL  |
| 37  | YR    | 67  | LEU  |
| 37  | YR    | 71  | GLN  |
| 37  | YR    | 75  | LEU  |
| 37  | YR    | 76  | VAL  |
| 37  | YR    | 81  | ASP  |
| 37  | YR    | 95  | THR  |
| 37  | YR    | 100 | LEU  |
| 37  | YR    | 104 | ARG  |
| 37  | YR    | 105 | ARG  |
| 37  | YR    | 107 | ASP  |
| 37  | YR    | 113 | LEU  |
| 38  | YS    | 4   | LEU  |
| 38  | YS    | 12  | PHE  |
| 38  | YS    | 17  | ARG  |
| 38  | YS    | 18  | ILE  |
| 38  | YS    | 20  | ARG  |
| 38  | YS    | 44  | LYS  |
| 38  | YS    | 56  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | YS    | 57  | LYS  |
| 38  | YS    | 73  | LEU  |
| 38  | YS    | 89  | ARG  |
| 38  | YS    | 101 | LEU  |
| 38  | YS    | 103 | GLU  |
| 38  | YS    | 106 | ARG  |
| 38  | YS    | 111 | GLU  |
| 39  | YT    | 2   | ASN  |
| 39  | YT    | 14  | TYR  |
| 39  | YT    | 22  | PHE  |
| 39  | YT    | 23  | ARG  |
| 39  | YT    | 27  | THR  |
| 39  | YT    | 42  | ILE  |
| 39  | YT    | 48  | ILE  |
| 39  | YT    | 50  | ILE  |
| 39  | YT    | 65  | LYS  |
| 39  | YT    | 73  | GLU  |
| 39  | YT    | 78  | LEU  |
| 39  | YT    | 86  | ILE  |
| 39  | YT    | 87  | ASP  |
| 39  | YT    | 100 | TYR  |
| 39  | YT    | 104 | ASN  |
| 39  | YT    | 107 | ASP  |
| 39  | YT    | 111 | ARG  |
| 39  | YT    | 112 | ARG  |
| 39  | YT    | 128 | GLU  |
| 39  | YT    | 134 | GLU  |
| 40  | YU    | 5   | LYS  |
| 40  | YU    | 9   | VAL  |
| 40  | YU    | 31  | SER  |
| 40  | YU    | 52  | ARG  |
| 40  | YU    | 60  | LEU  |
| 40  | YU    | 64  | ARG  |
| 40  | YU    | 79  | PHE  |
| 40  | YU    | 88  | ILE  |
| 40  | YU    | 92  | ARG  |
| 40  | YU    | 98  | LEU  |
| 40  | YU    | 108 | GLU  |
| 40  | YU    | 117 | GLN  |
| 41  | YV    | 14  | VAL  |
| 41  | YV    | 18  | LEU  |
| 41  | YV    | 24  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | YV    | 35  | LEU  |
| 41  | YV    | 37  | VAL  |
| 41  | YV    | 38  | LEU  |
| 41  | YV    | 39  | LEU  |
| 41  | YV    | 40  | LEU  |
| 41  | YV    | 47  | VAL  |
| 41  | YV    | 57  | VAL  |
| 41  | YV    | 61  | VAL  |
| 41  | YV    | 66  | ARG  |
| 41  | YV    | 70  | ILE  |
| 41  | YV    | 75  | PHE  |
| 41  | YV    | 91  | TYR  |
| 41  | YV    | 99  | ILE  |
| 42  | YW    | 11  | ARG  |
| 42  | YW    | 14  | PRO  |
| 42  | YW    | 16  | LYS  |
| 42  | YW    | 19  | LEU  |
| 42  | YW    | 20  | VAL  |
| 42  | YW    | 23  | LEU  |
| 42  | YW    | 63  | ASP  |
| 42  | YW    | 67  | ASP  |
| 42  | YW    | 69  | LEU  |
| 42  | YW    | 70  | TYR  |
| 42  | YW    | 87  | PRO  |
| 42  | YW    | 88  | ARG  |
| 42  | YW    | 92  | ARG  |
| 42  | YW    | 95  | ILE  |
| 42  | YW    | 107 | LEU  |
| 42  | YW    | 109 | GLU  |
| 43  | YX    | 3   | THR  |
| 43  | YX    | 15  | GLU  |
| 43  | YX    | 27  | THR  |
| 43  | YX    | 30  | VAL  |
| 43  | YX    | 49  | VAL  |
| 43  | YX    | 57  | LEU  |
| 43  | YX    | 65  | ARG  |
| 43  | YX    | 70  | LEU  |
| 43  | YX    | 72  | LYS  |
| 43  | YX    | 76  | ARG  |
| 43  | YX    | 80  | ILE  |
| 43  | YX    | 81  | VAL  |
| 43  | YX    | 88  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | YY    | 7   | VAL  |
| 44  | YY    | 26  | LYS  |
| 44  | YY    | 27  | VAL  |
| 44  | YY    | 42  | VAL  |
| 44  | YY    | 43  | ASN  |
| 44  | YY    | 45  | VAL  |
| 44  | YY    | 57  | GLN  |
| 44  | YY    | 61  | ILE  |
| 44  | YY    | 64  | GLU  |
| 44  | YY    | 72  | VAL  |
| 44  | YY    | 75  | ILE  |
| 44  | YY    | 77  | PRO  |
| 44  | YY    | 79  | CYS  |
| 44  | YY    | 87  | LYS  |
| 44  | YY    | 88  | 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    | 32  | HIS  |
| 45  | YZ    | 41  | LEU  |
| 45  | YZ    | 58  | VAL  |
| 45  | YZ    | 60  | GLU  |
| 45  | YZ    | 66  | SER  |
| 45  | YZ    | 70  | LEU  |
| 45  | YZ    | 71  | VAL  |
| 45  | YZ    | 76  | LEU  |
| 45  | YZ    | 87  | ASP  |
| 45  | YZ    | 91  | LEU  |
| 45  | YZ    | 94  | GLU  |
| 45  | YZ    | 123 | ASP  |
| 45  | YZ    | 133 | ILE  |
| 45  | YZ    | 139 | VAL  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | YZ    | 182 | LYS  |
| 45  | YZ    | 183 | LEU  |
| 46  | Y0    | 11  | ARG  |
| 46  | Y0    | 17  | GLN  |
| 46  | Y0    | 29  | GLN  |
| 46  | Y0    | 36  | ILE  |
| 46  | Y0    | 41  | ARG  |
| 46  | Y0    | 74  | ARG  |
| 47  | Y1    | 2   | SER  |
| 47  | Y1    | 11  | ARG  |
| 47  | Y1    | 30  | VAL  |
| 47  | Y1    | 41  | ARG  |
| 47  | Y1    | 56  | GLN  |
| 47  | Y1    | 75  | GLU  |
| 47  | Y1    | 80  | LEU  |
| 47  | Y1    | 81  | LYS  |
| 47  | Y1    | 83  | GLU  |
| 47  | Y1    | 87  | PRO  |
| 47  | Y1    | 91  | LYS  |
| 47  | Y1    | 97  | LEU  |
| 48  | Y2    | 7   | ARG  |
| 48  | Y2    | 9   | GLN  |
| 48  | Y2    | 16  | LEU  |
| 48  | Y2    | 24  | LEU  |
| 48  | Y2    | 47  | ASN  |
| 48  | Y2    | 53  | LEU  |
| 48  | Y2    | 62  | THR  |
| 48  | Y2    | 64  | LEU  |
| 49  | Y3    | 4   | LEU  |
| 49  | Y3    | 8   | LEU  |
| 49  | Y3    | 9   | VAL  |
| 49  | Y3    | 10  | LYS  |
| 49  | Y3    | 30  | ARG  |
| 49  | Y3    | 31  | LEU  |
| 49  | Y3    | 32  | GLN  |
| 49  | Y3    | 37  | LEU  |
| 49  | Y3    | 40  | THR  |
| 49  | Y3    | 44  | ARG  |
| 50  | Y4    | 6   | HIS  |
| 50  | Y4    | 15  | ILE  |
| 50  | Y4    | 18  | CYS  |
| 50  | Y4    | 21  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Y4    | 23  | GLU  |
| 50  | Y4    | 39  | CYS  |
| 50  | Y4    | 42  | PHE  |
| 50  | Y4    | 49  | PHE  |
| 50  | Y4    | 50  | VAL  |
| 50  | Y4    | 53  | GLU  |
| 50  | Y4    | 57  | GLU  |
| 50  | Y4    | 61  | ARG  |
| 50  | Y4    | 62  | ARG  |
| 50  | Y4    | 63  | TYR  |
| 50  | Y4    | 68  | ARG  |
| 50  | Y4    | 69  | LYS  |
| 50  | Y4    | 71  | ARG  |
| 51  | Y5    | 3   | LYS  |
| 51  | Y5    | 4   | HIS  |
| 51  | Y5    | 6   | VAL  |
| 51  | Y5    | 11  | THR  |
| 51  | Y5    | 19  | ARG  |
| 51  | Y5    | 25  | LEU  |
| 51  | Y5    | 36  | CYS  |
| 51  | Y5    | 37  | LYS  |
| 51  | Y5    | 52  | TYR  |
| 51  | Y5    | 56  | LYS  |
| 51  | Y5    | 58  | LEU  |
| 52  | Y6    | 6   | ARG  |
| 52  | Y6    | 8   | LYS  |
| 52  | Y6    | 10  | LEU  |
| 52  | Y6    | 18  | ARG  |
| 52  | Y6    | 19  | ARG  |
| 52  | Y6    | 27  | LYS  |
| 52  | Y6    | 33  | LYS  |
| 52  | Y6    | 34  | LEU  |
| 52  | Y6    | 37  | ARG  |
| 52  | Y6    | 42  | TRP  |
| 52  | Y6    | 44  | ARG  |
| 52  | Y6    | 53  | LYS  |
| 53  | Y7    | 1   | MET  |
| 53  | Y7    | 9   | ARG  |
| 53  | Y7    | 14  | LYS  |
| 53  | Y7    | 43  | THR  |
| 54  | Y8    | 16  | ILE  |
| 54  | Y8    | 30  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | Y8    | 35  | GLN  |
| 54  | Y8    | 39  | LYS  |
| 54  | Y8    | 43  | GLN  |
| 54  | Y8    | 47  | LYS  |
| 54  | Y8    | 48  | PHE  |
| 54  | Y8    | 49  | VAL  |
| 54  | Y8    | 52  | LYS  |
| 54  | Y8    | 53  | PRO  |
| 54  | Y8    | 59  | LYS  |
| 54  | Y8    | 62  | LEU  |
| 54  | Y8    | 63  | PRO  |
| 54  | Y8    | 65  | GLU  |
| 55  | Y9    | 1   | MET  |
| 55  | Y9    | 17  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 19  | HIS  |
| 2   | QB    | 95  | GLN  |
| 2   | QB    | 135 | GLN  |
| 2   | QB    | 204 | ASN  |
| 2   | QB    | 212 | GLN  |
| 2   | QB    | 224 | GLN  |
| 3   | QC    | 181 | ASN  |
| 4   | QD    | 43  | HIS  |
| 4   | QD    | 45  | GLN  |
| 4   | QD    | 74  | GLN  |
| 4   | QD    | 119 | GLN  |
| 5   | QE    | 72  | GLN  |
| 5   | QE    | 78  | HIS  |
| 6   | QF    | 64  | GLN  |
| 6   | QF    | 100 | ASN  |
| 7   | QG    | 28  | ASN  |
| 7   | QG    | 37  | ASN  |
| 7   | QG    | 86  | GLN  |
| 7   | QG    | 148 | ASN  |
| 8   | QH    | 78  | GLN  |
| 9   | QI    | 3   | GLN  |
| 9   | QI    | 73  | GLN  |
| 10  | QJ    | 76  | ASN  |
| 10  | QJ    | 78  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | QK    | 117 | ASN  |
| 12  | QL    | 9   | GLN  |
| 13  | QM    | 101 | GLN  |
| 19  | QS    | 65  | ASN  |
| 20  | QT    | 26  | ASN  |
| 27  | RD    | 44  | ASN  |
| 27  | RD    | 87  | ASN  |
| 27  | RD    | 112 | GLN  |
| 27  | RD    | 164 | GLN  |
| 27  | RD    | 166 | GLN  |
| 27  | RD    | 198 | ASN  |
| 28  | RE    | 35  | GLN  |
| 28  | RE    | 55  | ASN  |
| 28  | RE    | 180 | ASN  |
| 30  | RG    | 123 | ASN  |
| 31  | RH    | 143 | GLN  |
| 31  | RH    | 147 | ASN  |
| 31  | RH    | 158 | HIS  |
| 32  | RI    | 43  | ASN  |
| 33  | RN    | 56  | ASN  |
| 33  | RN    | 130 | HIS  |
| 33  | RN    | 131 | GLN  |
| 34  | RO    | 5   | GLN  |
| 34  | RO    | 82  | ASN  |
| 35  | RP    | 81  | GLN  |
| 35  | RP    | 84  | ASN  |
| 37  | RR    | 3   | HIS  |
| 37  | RR    | 61  | HIS  |
| 39  | RT    | 58  | ASN  |
| 39  | RT    | 90  | GLN  |
| 40  | RU    | 81  | HIS  |
| 40  | RU    | 94  | ASN  |
| 40  | RU    | 117 | GLN  |
| 41  | RV    | 11  | GLN  |
| 41  | RV    | 80  | GLN  |
| 41  | RV    | 87  | HIS  |
| 42  | RW    | 61  | ASN  |
| 43  | RX    | 55  | ASN  |
| 43  | RX    | 87  | GLN  |
| 44  | RY    | 57  | GLN  |
| 45  | RZ    | 73  | GLN  |
| 45  | RZ    | 132 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | R0    | 3   | HIS  |
| 47  | R1    | 56  | GLN  |
| 47  | R1    | 66  | HIS  |
| 48  | R2    | 47  | ASN  |
| 49  | R3    | 19  | GLN  |
| 49  | R3    | 32  | GLN  |
| 49  | R3    | 52  | HIS  |
| 52  | R6    | 26  | ASN  |
| 54  | R8    | 33  | ASN  |
| 55  | R9    | 34  | GLN  |
| 2   | XB    | 95  | GLN  |
| 2   | XB    | 204 | ASN  |
| 2   | XB    | 212 | GLN  |
| 2   | XB    | 224 | GLN  |
| 3   | XC    | 181 | ASN  |
| 4   | XD    | 43  | HIS  |
| 4   | XD    | 45  | GLN  |
| 4   | XD    | 119 | GLN  |
| 5   | XE    | 72  | GLN  |
| 5   | XE    | 78  | HIS  |
| 6   | XF    | 64  | GLN  |
| 6   | XF    | 100 | ASN  |
| 7   | XG    | 28  | ASN  |
| 7   | XG    | 37  | ASN  |
| 7   | XG    | 86  | GLN  |
| 7   | XG    | 148 | ASN  |
| 9   | XI    | 3   | GLN  |
| 9   | XI    | 31  | GLN  |
| 10  | XJ    | 76  | ASN  |
| 10  | XJ    | 78  | ASN  |
| 11  | XK    | 117 | ASN  |
| 12  | XL    | 9   | GLN  |
| 13  | XM    | 62  | ASN  |
| 13  | XM    | 77  | ASN  |
| 13  | XM    | 101 | GLN  |
| 15  | XO    | 62  | GLN  |
| 19  | XS    | 65  | ASN  |
| 20  | XT    | 26  | ASN  |
| 27  | YD    | 44  | ASN  |
| 27  | YD    | 87  | ASN  |
| 27  | YD    | 112 | GLN  |
| 27  | YD    | 164 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | YD    | 166 | GLN  |
| 27  | YD    | 198 | ASN  |
| 28  | YE    | 55  | ASN  |
| 28  | YE    | 180 | ASN  |
| 30  | YG    | 123 | ASN  |
| 31  | YH    | 143 | GLN  |
| 31  | YH    | 147 | ASN  |
| 31  | YH    | 158 | HIS  |
| 32  | YI    | 43  | ASN  |
| 33  | YN    | 56  | ASN  |
| 33  | YN    | 101 | HIS  |
| 33  | YN    | 130 | HIS  |
| 33  | YN    | 131 | GLN  |
| 34  | YO    | 5   | GLN  |
| 34  | YO    | 29  | ASN  |
| 34  | YO    | 82  | ASN  |
| 35  | YP    | 13  | ASN  |
| 35  | YP    | 81  | GLN  |
| 35  | YP    | 84  | ASN  |
| 37  | YR    | 61  | HIS  |
| 39  | YT    | 90  | GLN  |
| 40  | YU    | 94  | ASN  |
| 41  | YV    | 11  | GLN  |
| 41  | YV    | 80  | GLN  |
| 42  | YW    | 61  | ASN  |
| 42  | YW    | 102 | HIS  |
| 43  | YX    | 55  | ASN  |
| 43  | YX    | 87  | GLN  |
| 44  | YY    | 57  | GLN  |
| 45  | YZ    | 118 | GLN  |
| 45  | YZ    | 151 | HIS  |
| 46  | Y0    | 3   | HIS  |
| 46  | Y0    | 29  | GLN  |
| 47  | Y1    | 56  | GLN  |
| 47  | Y1    | 66  | HIS  |
| 48  | Y2    | 9   | GLN  |
| 48  | Y2    | 38  | GLN  |
| 48  | Y2    | 46  | GLN  |
| 48  | Y2    | 47  | ASN  |
| 49  | Y3    | 19  | GLN  |
| 49  | Y3    | 32  | GLN  |
| 49  | Y3    | 46  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | Y6    | 26  | ASN  |
| 54  | Y8    | 33  | ASN  |
| 55  | Y9    | 34  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1498/1522 (98%) | 269 (17%)         | 42 (2%)         |
| 1   | XA    | 1499/1522 (98%) | 289 (19%)         | 46 (3%)         |
| 22  | QV    | 76/77 (98%)     | 30 (39%)          | 1 (1%)          |
| 22  | XV    | 76/77 (98%)     | 30 (39%)          | 1 (1%)          |
| 23  | QY    | 14/17 (82%)     | 7 (50%)           | 1 (7%)          |
| 23  | XY    | 14/17 (82%)     | 7 (50%)           | 1 (7%)          |
| 24  | QX    | 7/25 (28%)      | 4 (57%)           | 1 (14%)         |
| 24  | XX    | 7/25 (28%)      | 4 (57%)           | 1 (14%)         |
| 25  | RA    | 2879/2916 (98%) | 620 (21%)         | 66 (2%)         |
| 25  | YA    | 2880/2916 (98%) | 623 (21%)         | 60 (2%)         |
| 26  | RB    | 119/122 (97%)   | 24 (20%)          | 2 (1%)          |
| 26  | YB    | 119/122 (97%)   | 24 (20%)          | 1 (0%)          |
| 56  | Z6    | 1/3 (33%)       | 0                 | 0               |
| 56  | Z8    | 1/3 (33%)       | 0                 | 0               |
| All | All   | 9190/9364 (98%) | 1931 (21%)        | 223 (2%)        |

All (1931) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 79  | G    |
| 1   | QA    | 80  | G    |
| 1   | QA    | 90  | C    |
| 1   | QA    | 91  | C    |
| 1   | QA    | 95  | G    |
| 1   | QA    | 101 | A    |
| 1   | QA    | 116 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 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    | 170    | U    |
| 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    | 201    | C    |
| 1   | QA    | 209    | U    |
| 1   | QA    | 210    | U    |
| 1   | QA    | 216    | G    |
| 1   | QA    | 231    | 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    | 278    | G    |
| 1   | QA    | 281    | G    |
| 1   | QA    | 289    | G    |
| 1   | QA    | 316    | 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    | 348    | G    |
| 1   | QA    | 351    | G    |
| 1   | QA    | 352    | C    |
| 1   | QA    | 353    | A    |
| 1   | QA    | 354    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 356 | A    |
| 1   | QA    | 367 | U    |
| 1   | QA    | 373 | A    |
| 1   | QA    | 388 | G    |
| 1   | QA    | 389 | A    |
| 1   | QA    | 397 | A    |
| 1   | QA    | 398 | C    |
| 1   | QA    | 406 | G    |
| 1   | QA    | 411 | A    |
| 1   | QA    | 412 | A    |
| 1   | QA    | 413 | G    |
| 1   | QA    | 421 | U    |
| 1   | QA    | 422 | C    |
| 1   | QA    | 423 | G    |
| 1   | QA    | 424 | G    |
| 1   | QA    | 429 | U    |
| 1   | QA    | 430 | A    |
| 1   | QA    | 440 | A    |
| 1   | QA    | 442 | C    |
| 1   | QA    | 452 | A    |
| 1   | QA    | 465 | A    |
| 1   | QA    | 466 | C    |
| 1   | QA    | 467 | G    |
| 1   | QA    | 468 | A    |
| 1   | QA    | 482 | A    |
| 1   | QA    | 485 | G    |
| 1   | QA    | 486 | U    |
| 1   | QA    | 496 | A    |
| 1   | QA    | 497 | U    |
| 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    | 547 | A    |
| 1   | QA    | 559 | A    |
| 1   | QA    | 561 | U    |
| 1   | QA    | 566 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 572 | A    |
| 1   | QA    | 573 | A    |
| 1   | QA    | 576 | G    |
| 1   | QA    | 577 | G    |
| 1   | QA    | 596 | C    |
| 1   | QA    | 614 | A    |
| 1   | QA    | 630 | G    |
| 1   | QA    | 631 | G    |
| 1   | QA    | 653 | A    |
| 1   | QA    | 686 | U    |
| 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    | 753 | A    |
| 1   | QA    | 754 | C    |
| 1   | QA    | 755 | G    |
| 1   | QA    | 777 | A    |
| 1   | QA    | 792 | A    |
| 1   | QA    | 793 | U    |
| 1   | QA    | 794 | A    |
| 1   | QA    | 813 | U    |
| 1   | QA    | 817 | C    |
| 1   | QA    | 818 | G    |
| 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    | 870 | U    |
| 1   | QA    | 871 | U    |
| 1   | QA    | 872 | A    |
| 1   | QA    | 885 | G    |
| 1   | QA    | 889 | A    |
| 1   | QA    | 902 | G    |
| 1   | QA    | 914 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 927     | G    |
| 1   | QA    | 934     | C    |
| 1   | QA    | 935     | A    |
| 1   | QA    | 960     | U    |
| 1   | QA    | 961     | U    |
| 1   | QA    | 966     | G    |
| 1   | QA    | 968     | A    |
| 1   | QA    | 969     | A    |
| 1   | QA    | 971     | G    |
| 1   | QA    | 974     | A    |
| 1   | QA    | 976     | G    |
| 1   | QA    | 977     | A    |
| 1   | QA    | 978     | A    |
| 1   | QA    | 980     | C    |
| 1   | QA    | 982     | U    |
| 1   | QA    | 991     | U    |
| 1   | QA    | 992     | U    |
| 1   | QA    | 993     | G    |
| 1   | QA    | 994     | A    |
| 1   | QA    | 1001    | G    |
| 1   | QA    | 1002    | G    |
| 1   | QA    | 1004    | A    |
| 1   | QA    | 1006    | C    |
| 1   | QA    | 1008    | 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    | 1054    | C    |
| 1   | QA    | 1064    | G    |
| 1   | QA    | 1065    | U    |
| 1   | QA    | 1066    | C    |
| 1   | QA    | 1094    | G    |
| 1   | QA    | 1095    | U    |
| 1   | QA    | 1101    | A    |
| 1   | QA    | 1124    | G    |
| 1   | QA    | 1125    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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    | 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    | 1200 | C    |
| 1   | QA    | 1201 | A    |
| 1   | QA    | 1202 | G    |
| 1   | QA    | 1212 | U    |
| 1   | QA    | 1213 | A    |
| 1   | QA    | 1225 | A    |
| 1   | QA    | 1238 | A    |
| 1   | QA    | 1240 | U    |
| 1   | QA    | 1241 | G    |
| 1   | QA    | 1256 | A    |
| 1   | QA    | 1257 | U    |
| 1   | QA    | 1258 | G    |
| 1   | QA    | 1270 | C    |
| 1   | QA    | 1273 | G    |
| 1   | QA    | 1280 | A    |
| 1   | QA    | 1281 | U    |
| 1   | QA    | 1282 | C    |
| 1   | QA    | 1286 | A    |
| 1   | QA    | 1287 | A    |
| 1   | QA    | 1290 | G    |
| 1   | QA    | 1296 | C    |
| 1   | QA    | 1297 | C    |
| 1   | QA    | 1298 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 1299    | A    |
| 1   | QA    | 1301    | U    |
| 1   | QA    | 1302    | U    |
| 1   | QA    | 1305    | G    |
| 1   | QA    | 1312    | G    |
| 1   | QA    | 1317    | C    |
| 1   | QA    | 1318    | 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    | 1338    | G    |
| 1   | QA    | 1347    | G    |
| 1   | QA    | 1348    | U    |
| 1   | QA    | 1353    | G    |
| 1   | QA    | 1362(A) | C    |
| 1   | QA    | 1363    | A    |
| 1   | QA    | 1364    | U    |
| 1   | QA    | 1370    | G    |
| 1   | QA    | 1397    | C    |
| 1   | QA    | 1401    | G    |
| 1   | QA    | 1419    | G    |
| 1   | QA    | 1442    | G    |
| 1   | QA    | 1446    | A    |
| 1   | QA    | 1447    | G    |
| 1   | QA    | 1452    | C    |
| 1   | QA    | 1453    | G    |
| 1   | QA    | 1454    | G    |
| 1   | QA    | 1492    | A    |
| 1   | QA    | 1497    | G    |
| 1   | QA    | 1499    | A    |
| 1   | QA    | 1502    | 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    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | QA    | 1529  | G    |
| 1   | QA    | 1530  | G    |
| 22  | QV    | 3     | C    |
| 22  | QV    | 4     | G    |
| 22  | QV    | 5     | G    |
| 22  | QV    | 7     | G    |
| 22  | QV    | 8     | U    |
| 22  | QV    | 14    | A    |
| 22  | QV    | 16    | C    |
| 22  | QV    | 17    | C    |
| 22  | QV    | 17(A) | U    |
| 22  | QV    | 18    | G    |
| 22  | QV    | 19    | G    |
| 22  | QV    | 21    | A    |
| 22  | QV    | 22    | G    |
| 22  | QV    | 25    | C    |
| 22  | QV    | 31    | G    |
| 22  | QV    | 37    | A    |
| 22  | QV    | 42    | G    |
| 22  | QV    | 47    | U    |
| 22  | QV    | 48    | C    |
| 22  | QV    | 49    | G    |
| 22  | QV    | 50    | U    |
| 22  | QV    | 51    | C    |
| 22  | QV    | 52    | G    |
| 22  | QV    | 54    | U    |
| 22  | QV    | 59    | A    |
| 22  | QV    | 63    | G    |
| 22  | QV    | 67    | C    |
| 22  | QV    | 72    | A    |
| 22  | QV    | 75    | C    |
| 22  | QV    | 76    | A    |
| 23  | QY    | 31    | G    |
| 23  | QY    | 32    | U    |
| 23  | QY    | 33    | U    |
| 23  | QY    | 34    | C    |
| 23  | QY    | 36    | G    |
| 23  | QY    | 41    | A    |
| 23  | QY    | 42    | G    |
| 24  | QX    | 3     | G    |
| 24  | QX    | 4     | C    |
| 24  | QX    | 7     | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | QX    | 8   | A    |
| 25  | RA    | 9   | U    |
| 25  | RA    | 11  | G    |
| 25  | RA    | 34  | C    |
| 25  | RA    | 46  | C    |
| 25  | RA    | 49  | A    |
| 25  | RA    | 51  | G    |
| 25  | RA    | 55  | G    |
| 25  | RA    | 72  | U    |
| 25  | RA    | 74  | A    |
| 25  | RA    | 75  | G    |
| 25  | RA    | 84  | A    |
| 25  | RA    | 96  | G    |
| 25  | RA    | 97  | C    |
| 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    | 188 | G    |
| 25  | RA    | 196 | A    |
| 25  | RA    | 199 | A    |
| 25  | RA    | 215 | G    |
| 25  | RA    | 216 | A    |
| 25  | RA    | 221 | A    |
| 25  | RA    | 222 | A    |
| 25  | RA    | 223 | A    |
| 25  | RA    | 228 | A    |
| 25  | RA    | 229 | A    |
| 25  | RA    | 230 | U    |
| 25  | RA    | 232 | G    |
| 25  | RA    | 241 | 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    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 265    | A    |
| 25  | RA    | 266    | G    |
| 25  | RA    | 268    | C    |
| 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    | 270(Z) | U    |
| 25  | RA    | 271(B) | G    |
| 25  | RA    | 271(C) | U    |
| 25  | RA    | 271    | G    |
| 25  | RA    | 273(F) | C    |
| 25  | RA    | 275    | G    |
| 25  | RA    | 276    | A    |
| 25  | RA    | 277    | C    |
| 25  | RA    | 278    | A    |
| 25  | RA    | 299    | A    |
| 25  | RA    | 311    | A    |
| 25  | RA    | 316    | C    |
| 25  | RA    | 323    | G    |
| 25  | RA    | 324    | A    |
| 25  | RA    | 329    | G    |
| 25  | RA    | 330    | A    |
| 25  | RA    | 333    | G    |
| 25  | RA    | 335    | C    |
| 25  | RA    | 342    | G    |
| 25  | RA    | 346    | A    |
| 25  | RA    | 352    | G    |
| 25  | RA    | 363(F) | A    |
| 25  | RA    | 364    | C    |
| 25  | RA    | 371    | A    |
| 25  | RA    | 372    | G    |
| 25  | RA    | 373    | U    |
| 25  | RA    | 386    | G    |
| 25  | RA    | 395    | U    |
| 25  | RA    | 405    | U    |
| 25  | RA    | 411    | G    |
| 25  | RA    | 412    | A    |
| 25  | RA    | 428    | A    |
| 25  | RA    | 442    | G    |
| 25  | RA    | 444    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | RA    | 448 | U    |
| 25  | RA    | 449 | A    |
| 25  | RA    | 454 | A    |
| 25  | RA    | 457 | A    |
| 25  | RA    | 470 | A    |
| 25  | RA    | 481 | G    |
| 25  | RA    | 484 | C    |
| 25  | RA    | 494 | G    |
| 25  | RA    | 503 | A    |
| 25  | RA    | 504 | U    |
| 25  | RA    | 505 | A    |
| 25  | RA    | 509 | C    |
| 25  | RA    | 512 | G    |
| 25  | RA    | 513 | A    |
| 25  | RA    | 518 | G    |
| 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    | 549 | G    |
| 25  | RA    | 554 | U    |
| 25  | RA    | 556 | G    |
| 25  | RA    | 563 | G    |
| 25  | RA    | 573 | G    |
| 25  | RA    | 574 | C    |
| 25  | RA    | 575 | A    |
| 25  | RA    | 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    | 627 | A    |
| 25  | RA    | 637 | A    |
| 25  | RA    | 638 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 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    | 654(B) | C    |
| 25  | RA    | 659    | C    |
| 25  | RA    | 669    | G    |
| 25  | RA    | 686    | G    |
| 25  | RA    | 702    | G    |
| 25  | RA    | 705    | A    |
| 25  | RA    | 717    | G    |
| 25  | RA    | 722    | A    |
| 25  | RA    | 730    | C    |
| 25  | RA    | 747    | U    |
| 25  | RA    | 753    | C    |
| 25  | RA    | 764    | A    |
| 25  | RA    | 775    | G    |
| 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    | 791    | C    |
| 25  | RA    | 792    | G    |
| 25  | RA    | 805    | G    |
| 25  | RA    | 812    | C    |
| 25  | RA    | 819    | A    |
| 25  | RA    | 827    | U    |
| 25  | RA    | 828    | U    |
| 25  | RA    | 846    | C    |
| 25  | RA    | 847    | U    |
| 25  | RA    | 854    | G    |
| 25  | RA    | 856    | C    |
| 25  | RA    | 857    | C    |
| 25  | RA    | 859    | G    |
| 25  | RA    | 860    | U    |
| 25  | RA    | 865    | C    |
| 25  | RA    | 869    | G    |
| 25  | RA    | 880    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 881    | G    |
| 25  | RA    | 882    | 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    | 938    | G    |
| 25  | RA    | 941    | A    |
| 25  | RA    | 945    | A    |
| 25  | RA    | 946    | G    |
| 25  | RA    | 961    | C    |
| 25  | RA    | 973    | A    |
| 25  | RA    | 974    | G    |
| 25  | RA    | 974(A) | C    |
| 25  | RA    | 975    | G    |
| 25  | RA    | 983    | A    |
| 25  | RA    | 990    | A    |
| 25  | RA    | 991    | C    |
| 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    | 1020   | A    |
| 25  | RA    | 1023   | U    |
| 25  | RA    | 1025   | G    |
| 25  | RA    | 1026   | U    |
| 25  | RA    | 1027   | A    |
| 25  | RA    | 1033   | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1044       | G           |
| 25         | RA           | 1045       | A           |
| 25         | RA           | 1046       | A           |
| 25         | RA           | 1050       | 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           | 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           |
| 25         | RA           | 1082       | U           |
| 25         | RA           | 1083       | U           |
| 25         | RA           | 1084       | A           |
| 25         | RA           | 1085       | A           |
| 25         | RA           | 1086       | A           |
| 25         | RA           | 1088       | A           |
| 25         | RA           | 1090       | U           |
| 25         | RA           | 1091       | G           |
| 25         | RA           | 1093       | G           |
| 25         | RA           | 1095       | A           |
| 25         | RA           | 1096       | A           |
| 25         | RA           | 1104       | C           |
| 25         | RA           | 1105       | U           |
| 25         | RA           | 1110       | G           |
| 25         | RA           | 1111       | A           |
| 25         | RA           | 1112       | G           |
| 25         | RA           | 1122       | G           |
| 25         | RA           | 1128       | A           |
| 25         | RA           | 1129       | A           |
| 25         | RA           | 1131       | G           |
| 25         | RA           | 1135       | C           |
| 25         | RA           | 1136       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 1142    | U    |
| 25  | RA    | 1142(A) | A    |
| 25  | RA    | 1151    | G    |
| 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    | 1186    | 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    | 1236    | G    |
| 25  | RA    | 1238    | G    |
| 25  | RA    | 1248    | G    |
| 25  | RA    | 1253    | A    |
| 25  | RA    | 1256    | G    |
| 25  | RA    | 1265    | A    |
| 25  | RA    | 1271    | G    |
| 25  | RA    | 1272    | A    |
| 25  | RA    | 1273    | U    |
| 25  | RA    | 1300    | U    |
| 25  | RA    | 1301    | A    |
| 25  | RA    | 1304    | C    |
| 25  | RA    | 1306    | C    |
| 25  | RA    | 1309    | G    |
| 25  | RA    | 1312    | U    |
| 25  | RA    | 1313    | U    |
| 25  | RA    | 1314    | C    |
| 25  | RA    | 1319    | G    |
| 25  | RA    | 1321    | A    |
| 25  | RA    | 1329    | U    |
| 25  | RA    | 1332    | G    |
| 25  | RA    | 1349    | A    |
| 25  | RA    | 1352    | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 1365    | A    |
| 25  | RA    | 1368    | G    |
| 25  | RA    | 1372    | U    |
| 25  | RA    | 1379    | A    |
| 25  | RA    | 1380    | G    |
| 25  | RA    | 1384    | A    |
| 25  | RA    | 1385    | G    |
| 25  | RA    | 1386    | C    |
| 25  | RA    | 1391    | U    |
| 25  | RA    | 1395    | A    |
| 25  | RA    | 1396    | U    |
| 25  | RA    | 1407    | C    |
| 25  | RA    | 1411    | C    |
| 25  | RA    | 1413    | G    |
| 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    | 1460    | A    |
| 25  | RA    | 1461    | G    |
| 25  | RA    | 1467    | C    |
| 25  | RA    | 1471    | A    |
| 25  | RA    | 1473    | G    |
| 25  | RA    | 1474    | C    |
| 25  | RA    | 1482    | U    |
| 25  | RA    | 1483    | G    |
| 25  | RA    | 1485    | G    |
| 25  | RA    | 1491    | G    |
| 25  | RA    | 1493    | C    |
| 25  | RA    | 1497    | U    |
| 25  | RA    | 1504    | C    |
| 25  | RA    | 1505    | C    |
| 25  | RA    | 1506    | C    |
| 25  | RA    | 1507    | A    |
| 25  | RA    | 1508    | A    |
| 25  | RA    | 1510    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 1511 | A    |
| 25  | RA    | 1514 | U    |
| 25  | RA    | 1522 | G    |
| 25  | RA    | 1525 | 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    | 1566 | A    |
| 25  | RA    | 1569 | A    |
| 25  | RA    | 1578 | U    |
| 25  | RA    | 1579 | A    |
| 25  | RA    | 1581 | G    |
| 25  | RA    | 1585 | C    |
| 25  | RA    | 1586 | A    |
| 25  | RA    | 1591 | G    |
| 25  | RA    | 1598 | C    |
| 25  | RA    | 1608 | A    |
| 25  | RA    | 1609 | A    |
| 25  | RA    | 1610 | A    |
| 25  | RA    | 1616 | A    |
| 25  | RA    | 1617 | C    |
| 25  | RA    | 1618 | A    |
| 25  | RA    | 1648 | C    |
| 25  | RA    | 1654 | A    |
| 25  | RA    | 1667 | G    |
| 25  | RA    | 1668 | A    |
| 25  | RA    | 1669 | A    |
| 25  | RA    | 1674 | G    |
| 25  | RA    | 1694 | C    |
| 25  | RA    | 1695 | G    |
| 25  | RA    | 1725 | G    |
| 25  | RA    | 1729 | A    |
| 25  | RA    | 1730 | U    |
| 25  | RA    | 1731 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 1733 | G    |
| 25  | RA    | 1742 | C    |
| 25  | RA    | 1743 | G    |
| 25  | RA    | 1754 | C    |
| 25  | RA    | 1756 | G    |
| 25  | RA    | 1763 | G    |
| 25  | RA    | 1764 | G    |
| 25  | RA    | 1769 | G    |
| 25  | RA    | 1773 | A    |
| 25  | RA    | 1780 | A    |
| 25  | RA    | 1782 | C    |
| 25  | RA    | 1787 | A    |
| 25  | RA    | 1791 | A    |
| 25  | RA    | 1799 | G    |
| 25  | RA    | 1800 | C    |
| 25  | RA    | 1801 | G    |
| 25  | RA    | 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    | 1860 | 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    | 1896 | G    |
| 25  | RA    | 1903 | G    |
| 25  | RA    | 1905 | C    |
| 25  | RA    | 1906 | G    |
| 25  | RA    | 1913 | A    |
| 25  | RA    | 1929 | G    |
| 25  | RA    | 1930 | G    |
| 25  | RA    | 1931 | U    |
| 25  | RA    | 1937 | A    |
| 25  | RA    | 1938 | A    |
| 25  | RA    | 1939 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 1946 | U    |
| 25  | RA    | 1955 | U    |
| 25  | RA    | 1963 | U    |
| 25  | RA    | 1967 | C    |
| 25  | RA    | 1969 | A    |
| 25  | RA    | 1970 | A    |
| 25  | RA    | 1971 | A    |
| 25  | RA    | 1972 | A    |
| 25  | RA    | 1981 | A    |
| 25  | RA    | 1982 | C    |
| 25  | RA    | 1991 | U    |
| 25  | RA    | 1992 | G    |
| 25  | RA    | 1993 | U    |
| 25  | RA    | 2004 | G    |
| 25  | RA    | 2021 | C    |
| 25  | RA    | 2023 | G    |
| 25  | RA    | 2031 | A    |
| 25  | RA    | 2032 | G    |
| 25  | RA    | 2033 | A    |
| 25  | RA    | 2043 | C    |
| 25  | RA    | 2051 | A    |
| 25  | RA    | 2052 | G    |
| 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    | 2096 | U    |
| 25  | RA    | 2111 | C    |
| 25  | RA    | 2113 | U    |
| 25  | RA    | 2114 | A    |
| 25  | RA    | 2115 | G    |
| 25  | RA    | 2116 | G    |
| 25  | RA    | 2117 | A    |
| 25  | RA    | 2118 | U    |
| 25  | RA    | 2120 | G    |
| 25  | RA    | 2126 | A    |
| 25  | RA    | 2127 | G    |
| 25  | RA    | 2128 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2131 | G    |
| 25  | RA    | 2132 | U    |
| 25  | RA    | 2133 | G    |
| 25  | RA    | 2136 | C    |
| 25  | RA    | 2146 | C    |
| 25  | RA    | 2148 | G    |
| 25  | RA    | 2158 | A    |
| 25  | RA    | 2161 | C    |
| 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    | 2235 | G    |
| 25  | RA    | 2239 | G    |
| 25  | RA    | 2243 | U    |
| 25  | RA    | 2275 | C    |
| 25  | RA    | 2283 | C    |
| 25  | RA    | 2287 | A    |
| 25  | RA    | 2288 | A    |
| 25  | RA    | 2305 | A    |
| 25  | RA    | 2307 | G    |
| 25  | RA    | 2308 | G    |
| 25  | RA    | 2310 | A    |
| 25  | RA    | 2311 | A    |
| 25  | RA    | 2314 | C    |
| 25  | RA    | 2319 | G    |
| 25  | RA    | 2320 | A    |
| 25  | RA    | 2321 | G    |
| 25  | RA    | 2325 | G    |
| 25  | RA    | 2326 | C    |
| 25  | RA    | 2334 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2342 | C    |
| 25  | RA    | 2345 | G    |
| 25  | RA    | 2346 | A    |
| 25  | RA    | 2347 | C    |
| 25  | RA    | 2358 | G    |
| 25  | RA    | 2372 | G    |
| 25  | RA    | 2382 | G    |
| 25  | RA    | 2383 | G    |
| 25  | RA    | 2385 | C    |
| 25  | RA    | 2394 | C    |
| 25  | RA    | 2397 | G    |
| 25  | RA    | 2400 | G    |
| 25  | RA    | 2402 | C    |
| 25  | RA    | 2403 | C    |
| 25  | RA    | 2406 | U    |
| 25  | RA    | 2410 | G    |
| 25  | RA    | 2423 | U    |
| 25  | RA    | 2425 | A    |
| 25  | RA    | 2429 | G    |
| 25  | RA    | 2430 | A    |
| 25  | RA    | 2434 | A    |
| 25  | RA    | 2435 | A    |
| 25  | RA    | 2439 | A    |
| 25  | RA    | 2440 | C    |
| 25  | RA    | 2441 | C    |
| 25  | RA    | 2445 | G    |
| 25  | RA    | 2448 | A    |
| 25  | RA    | 2450 | A    |
| 25  | RA    | 2452 | C    |
| 25  | RA    | 2469 | A    |
| 25  | RA    | 2470 | G    |
| 25  | RA    | 2475 | C    |
| 25  | RA    | 2476 | A    |
| 25  | RA    | 2481 | G    |
| 25  | RA    | 2482 | G    |
| 25  | RA    | 2483 | C    |
| 25  | RA    | 2484 | G    |
| 25  | RA    | 2494 | G    |
| 25  | RA    | 2497 | A    |
| 25  | RA    | 2499 | C    |
| 25  | RA    | 2502 | G    |
| 25  | RA    | 2505 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 2506    | U    |
| 25  | RA    | 2507    | C    |
| 25  | RA    | 2519    | U    |
| 25  | RA    | 2529    | G    |
| 25  | RA    | 2542    | A    |
| 25  | RA    | 2543    | G    |
| 25  | RA    | 2554    | U    |
| 25  | RA    | 2560    | C    |
| 25  | RA    | 2566    | A    |
| 25  | RA    | 2567    | G    |
| 25  | RA    | 2569    | G    |
| 25  | RA    | 2573    | C    |
| 25  | RA    | 2578    | G    |
| 25  | RA    | 2591    | C    |
| 25  | RA    | 2602    | A    |
| 25  | RA    | 2609    | U    |
| 25  | RA    | 2610    | C    |
| 25  | RA    | 2611    | U    |
| 25  | RA    | 2612    | C    |
| 25  | RA    | 2614    | A    |
| 25  | RA    | 2623    | G    |
| 25  | RA    | 2629    | A    |
| 25  | RA    | 2646    | C    |
| 25  | RA    | 2655    | G    |
| 25  | RA    | 2665    | A    |
| 25  | RA    | 2673    | G    |
| 25  | RA    | 2675    | A    |
| 25  | RA    | 2682    | U    |
| 25  | RA    | 2689    | U    |
| 25  | RA    | 2690    | C    |
| 25  | RA    | 2702    | U    |
| 25  | RA    | 2703    | C    |
| 25  | RA    | 2712    | U    |
| 25  | RA    | 2712(A) | A    |
| 25  | RA    | 2713    | A    |
| 25  | RA    | 2714    | G    |
| 25  | RA    | 2724    | C    |
| 25  | RA    | 2726    | U    |
| 25  | RA    | 2733    | A    |
| 25  | RA    | 2734    | A    |
| 25  | RA    | 2748    | A    |
| 25  | RA    | 2752    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2757 | A    |
| 25  | RA    | 2758 | A    |
| 25  | RA    | 2761 | G    |
| 25  | RA    | 2764 | A    |
| 25  | RA    | 2765 | A    |
| 25  | RA    | 2766 | G    |
| 25  | RA    | 2770 | G    |
| 25  | RA    | 2771 | C    |
| 25  | RA    | 2777 | G    |
| 25  | RA    | 2778 | A    |
| 25  | RA    | 2779 | U    |
| 25  | RA    | 2780 | G    |
| 25  | RA    | 2781 | A    |
| 25  | RA    | 2790 | A    |
| 25  | RA    | 2791 | C    |
| 25  | RA    | 2797 | U    |
| 25  | RA    | 2807 | G    |
| 25  | RA    | 2818 | G    |
| 25  | RA    | 2820 | A    |
| 25  | RA    | 2821 | A    |
| 25  | RA    | 2833 | G    |
| 25  | RA    | 2834 | G    |
| 25  | RA    | 2839 | G    |
| 25  | RA    | 2846 | G    |
| 25  | RA    | 2849 | U    |
| 25  | RA    | 2867 | G    |
| 25  | RA    | 2868 | A    |
| 25  | RA    | 2872 | G    |
| 25  | RA    | 2874 | 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    | 21   | G    |
| 26  | RB    | 22   | U    |
| 26  | RB    | 25   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | RB    | 32  | C    |
| 26  | RB    | 33  | G    |
| 26  | RB    | 34  | U    |
| 26  | RB    | 35  | U    |
| 26  | RB    | 42  | C    |
| 26  | RB    | 45  | A    |
| 26  | RB    | 52  | A    |
| 26  | RB    | 53  | A    |
| 26  | RB    | 56  | G    |
| 26  | RB    | 57  | A    |
| 26  | RB    | 67  | G    |
| 26  | RB    | 73  | A    |
| 26  | RB    | 81  | G    |
| 26  | RB    | 82  | G    |
| 26  | RB    | 109 | G    |
| 1   | XA    | 6   | G    |
| 1   | XA    | 8   | A    |
| 1   | XA    | 32  | A    |
| 1   | XA    | 39  | G    |
| 1   | XA    | 47  | C    |
| 1   | XA    | 48  | C    |
| 1   | XA    | 51  | A    |
| 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    | 116 | A    |
| 1   | XA    | 120 | A    |
| 1   | XA    | 121 | C    |
| 1   | XA    | 130 | A    |
| 1   | XA    | 144 | G    |
| 1   | XA    | 147 | G    |
| 1   | XA    | 163 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | XA    | 172    | A    |
| 1   | XA    | 173    | U    |
| 1   | XA    | 174    | C    |
| 1   | XA    | 182    | U    |
| 1   | XA    | 190    | G    |
| 1   | XA    | 191(A) | G    |
| 1   | XA    | 195    | A    |
| 1   | XA    | 197    | A    |
| 1   | XA    | 201    | C    |
| 1   | XA    | 209    | U    |
| 1   | XA    | 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    |
| 1   | XA    | 270    | A    |
| 1   | XA    | 281    | G    |
| 1   | XA    | 289    | G    |
| 1   | XA    | 315    | A    |
| 1   | XA    | 316    | G    |
| 1   | XA    | 321    | A    |
| 1   | XA    | 328    | C    |
| 1   | XA    | 329    | A    |
| 1   | XA    | 330    | C    |
| 1   | XA    | 332    | G    |
| 1   | XA    | 345    | C    |
| 1   | XA    | 346    | G    |
| 1   | XA    | 347    | G    |
| 1   | XA    | 348    | G    |
| 1   | XA    | 349    | A    |
| 1   | XA    | 352    | C    |
| 1   | XA    | 353    | A    |
| 1   | XA    | 354    | G    |
| 1   | XA    | 356    | A    |
| 1   | XA    | 367    | U    |
| 1   | XA    | 373    | A    |
| 1   | XA    | 384    | G    |
| 1   | XA    | 388    | G    |
| 1   | XA    | 390    | C    |
| 1   | XA    | 392    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 397 | A    |
| 1   | XA    | 398 | C    |
| 1   | XA    | 411 | A    |
| 1   | XA    | 412 | A    |
| 1   | XA    | 413 | G    |
| 1   | XA    | 414 | A    |
| 1   | XA    | 422 | C    |
| 1   | XA    | 423 | G    |
| 1   | XA    | 424 | G    |
| 1   | XA    | 428 | G    |
| 1   | XA    | 429 | U    |
| 1   | XA    | 430 | A    |
| 1   | XA    | 440 | A    |
| 1   | XA    | 466 | C    |
| 1   | XA    | 467 | G    |
| 1   | XA    | 482 | A    |
| 1   | XA    | 485 | G    |
| 1   | XA    | 486 | U    |
| 1   | XA    | 496 | A    |
| 1   | XA    | 497 | U    |
| 1   | XA    | 509 | A    |
| 1   | XA    | 510 | A    |
| 1   | XA    | 511 | C    |
| 1   | XA    | 518 | C    |
| 1   | XA    | 521 | G    |
| 1   | XA    | 527 | G    |
| 1   | XA    | 531 | U    |
| 1   | XA    | 532 | A    |
| 1   | XA    | 533 | A    |
| 1   | XA    | 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    | 595 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 596 | C    |
| 1   | XA    | 615 | C    |
| 1   | XA    | 619 | U    |
| 1   | XA    | 630 | G    |
| 1   | XA    | 631 | G    |
| 1   | XA    | 632 | A    |
| 1   | XA    | 633 | G    |
| 1   | XA    | 653 | A    |
| 1   | XA    | 665 | A    |
| 1   | XA    | 686 | U    |
| 1   | XA    | 688 | G    |
| 1   | XA    | 701 | C    |
| 1   | XA    | 702 | A    |
| 1   | XA    | 704 | A    |
| 1   | XA    | 721 | G    |
| 1   | XA    | 723 | U    |
| 1   | XA    | 729 | A    |
| 1   | XA    | 731 | G    |
| 1   | XA    | 749 | C    |
| 1   | XA    | 753 | A    |
| 1   | XA    | 754 | C    |
| 1   | XA    | 755 | G    |
| 1   | XA    | 774 | G    |
| 1   | XA    | 777 | A    |
| 1   | XA    | 786 | G    |
| 1   | XA    | 792 | A    |
| 1   | XA    | 793 | U    |
| 1   | XA    | 794 | A    |
| 1   | XA    | 813 | U    |
| 1   | XA    | 816 | A    |
| 1   | XA    | 817 | C    |
| 1   | XA    | 818 | G    |
| 1   | XA    | 819 | A    |
| 1   | XA    | 821 | G    |
| 1   | XA    | 828 | A    |
| 1   | XA    | 841 | U    |
| 1   | XA    | 843 | U    |
| 1   | XA    | 848 | C    |
| 1   | XA    | 859 | A    |
| 1   | XA    | 870 | U    |
| 1   | XA    | 871 | U    |
| 1   | XA    | 872 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 891     | U    |
| 1   | XA    | 902     | G    |
| 1   | XA    | 914     | A    |
| 1   | XA    | 920     | U    |
| 1   | XA    | 926     | G    |
| 1   | XA    | 927     | G    |
| 1   | XA    | 934     | C    |
| 1   | XA    | 935     | A    |
| 1   | XA    | 960     | U    |
| 1   | XA    | 961     | U    |
| 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    | 983     | A    |
| 1   | XA    | 991     | U    |
| 1   | XA    | 992     | U    |
| 1   | XA    | 993     | G    |
| 1   | XA    | 1001    | G    |
| 1   | XA    | 1004    | A    |
| 1   | XA    | 1005    | A    |
| 1   | XA    | 1006    | C    |
| 1   | XA    | 1008    | C    |
| 1   | XA    | 1021    | G    |
| 1   | XA    | 1024    | G    |
| 1   | XA    | 1025    | U    |
| 1   | XA    | 1028    | C    |
| 1   | XA    | 1029    | G    |
| 1   | XA    | 1030    | C    |
| 1   | XA    | 1032(A) | G    |
| 1   | XA    | 1036    | G    |
| 1   | XA    | 1040    | U    |
| 1   | XA    | 1054    | C    |
| 1   | XA    | 1055    | A    |
| 1   | XA    | 1066    | C    |
| 1   | XA    | 1094    | G    |
| 1   | XA    | 1095    | U    |
| 1   | XA    | 1101    | A    |
| 1   | XA    | 1104    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | XA    | 1124 | G    |
| 1   | XA    | 1125 | U    |
| 1   | XA    | 1126 | U    |
| 1   | XA    | 1127 | G    |
| 1   | XA    | 1130 | A    |
| 1   | XA    | 1131 | G    |
| 1   | XA    | 1136 | U    |
| 1   | XA    | 1137 | C    |
| 1   | XA    | 1138 | G    |
| 1   | XA    | 1139 | G    |
| 1   | XA    | 1146 | A    |
| 1   | XA    | 1157 | A    |
| 1   | XA    | 1158 | C    |
| 1   | XA    | 1159 | U    |
| 1   | XA    | 1160 | G    |
| 1   | XA    | 1162 | C    |
| 1   | XA    | 1171 | G    |
| 1   | XA    | 1176 | A    |
| 1   | XA    | 1177 | G    |
| 1   | XA    | 1181 | G    |
| 1   | XA    | 1182 | G    |
| 1   | XA    | 1183 | A    |
| 1   | XA    | 1195 | C    |
| 1   | XA    | 1196 | U    |
| 1   | XA    | 1200 | C    |
| 1   | XA    | 1201 | A    |
| 1   | XA    | 1202 | G    |
| 1   | XA    | 1212 | U    |
| 1   | XA    | 1214 | C    |
| 1   | XA    | 1225 | A    |
| 1   | XA    | 1227 | A    |
| 1   | XA    | 1236 | 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    | 1270 | C    |
| 1   | XA    | 1273 | G    |
| 1   | XA    | 1280 | A    |
| 1   | XA    | 1281 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1286    | A    |
| 1   | XA    | 1287    | A    |
| 1   | XA    | 1297    | C    |
| 1   | XA    | 1298    | C    |
| 1   | XA    | 1299    | A    |
| 1   | XA    | 1300    | G    |
| 1   | XA    | 1301    | U    |
| 1   | XA    | 1302    | U    |
| 1   | XA    | 1303    | C    |
| 1   | XA    | 1305    | G    |
| 1   | XA    | 1317    | C    |
| 1   | XA    | 1318    | A    |
| 1   | XA    | 1319    | A    |
| 1   | XA    | 1320    | C    |
| 1   | XA    | 1321    | C    |
| 1   | XA    | 1322    | C    |
| 1   | XA    | 1323    | G    |
| 1   | XA    | 1331    | G    |
| 1   | XA    | 1332    | A    |
| 1   | XA    | 1335    | C    |
| 1   | XA    | 1336    | C    |
| 1   | XA    | 1338    | G    |
| 1   | XA    | 1347    | G    |
| 1   | XA    | 1353    | G    |
| 1   | XA    | 1362(A) | C    |
| 1   | XA    | 1363    | A    |
| 1   | XA    | 1364    | U    |
| 1   | XA    | 1365    | G    |
| 1   | XA    | 1370    | G    |
| 1   | XA    | 1397    | C    |
| 1   | XA    | 1398    | A    |
| 1   | XA    | 1419    | G    |
| 1   | XA    | 1442    | G    |
| 1   | XA    | 1443    | 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    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | XA    | 1499  | A    |
| 1   | XA    | 1502  | A    |
| 1   | XA    | 1503  | A    |
| 1   | XA    | 1504  | 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     | C    |
| 22  | XV    | 4     | G    |
| 22  | XV    | 5     | G    |
| 22  | XV    | 7     | G    |
| 22  | XV    | 8     | U    |
| 22  | XV    | 14    | A    |
| 22  | XV    | 16    | C    |
| 22  | XV    | 17    | C    |
| 22  | XV    | 17(A) | U    |
| 22  | XV    | 18    | G    |
| 22  | XV    | 19    | G    |
| 22  | XV    | 21    | A    |
| 22  | XV    | 22    | G    |
| 22  | XV    | 25    | C    |
| 22  | XV    | 31    | G    |
| 22  | XV    | 37    | A    |
| 22  | XV    | 42    | G    |
| 22  | XV    | 47    | U    |
| 22  | XV    | 48    | C    |
| 22  | XV    | 49    | G    |
| 22  | XV    | 50    | U    |
| 22  | XV    | 51    | C    |
| 22  | XV    | 52    | G    |
| 22  | XV    | 54    | U    |
| 22  | XV    | 59    | A    |
| 22  | XV    | 63    | G    |
| 22  | XV    | 67    | C    |
| 22  | XV    | 72    | A    |
| 22  | XV    | 75    | C    |
| 22  | XV    | 76    | A    |
| 23  | XY    | 31    | G    |
| 23  | XY    | 32    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | XY    | 33  | U    |
| 23  | XY    | 34  | C    |
| 23  | XY    | 36  | G    |
| 23  | XY    | 41  | A    |
| 23  | XY    | 42  | G    |
| 24  | XX    | 3   | G    |
| 24  | XX    | 4   | C    |
| 24  | XX    | 7   | G    |
| 24  | XX    | 8   | A    |
| 25  | YA    | 9   | U    |
| 25  | YA    | 15  | G    |
| 25  | YA    | 27  | G    |
| 25  | YA    | 34  | C    |
| 25  | YA    | 35  | G    |
| 25  | YA    | 46  | C    |
| 25  | YA    | 55  | G    |
| 25  | YA    | 61  | G    |
| 25  | YA    | 63  | U    |
| 25  | YA    | 64  | A    |
| 25  | YA    | 72  | U    |
| 25  | YA    | 74  | A    |
| 25  | YA    | 75  | G    |
| 25  | YA    | 98  | G    |
| 25  | YA    | 99  | U    |
| 25  | YA    | 101 | G    |
| 25  | YA    | 102 | G    |
| 25  | YA    | 103 | A    |
| 25  | YA    | 118 | A    |
| 25  | YA    | 119 | A    |
| 25  | YA    | 120 | U    |
| 25  | YA    | 125 | G    |
| 25  | YA    | 131 | G    |
| 25  | YA    | 161 | U    |
| 25  | YA    | 162 | U    |
| 25  | YA    | 177 | G    |
| 25  | YA    | 181 | A    |
| 25  | YA    | 195 | A    |
| 25  | YA    | 196 | A    |
| 25  | YA    | 199 | A    |
| 25  | YA    | 205 | G    |
| 25  | YA    | 206 | U    |
| 25  | YA    | 214 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 216    | A    |
| 25  | YA    | 221    | A    |
| 25  | YA    | 222    | A    |
| 25  | YA    | 223    | A    |
| 25  | YA    | 228    | A    |
| 25  | YA    | 229    | A    |
| 25  | YA    | 230    | U    |
| 25  | YA    | 232    | G    |
| 25  | YA    | 233    | A    |
| 25  | YA    | 242    | G    |
| 25  | YA    | 243    | U    |
| 25  | YA    | 248    | G    |
| 25  | YA    | 249    | C    |
| 25  | YA    | 250    | 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    | 285    | C    |
| 25  | YA    | 287    | C    |
| 25  | YA    | 299    | A    |
| 25  | YA    | 300    | A    |
| 25  | YA    | 305    | U    |
| 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | YA    | 352 | G    |
| 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    | 411 | G    |
| 25  | YA    | 412 | A    |
| 25  | YA    | 421 | U    |
| 25  | YA    | 428 | A    |
| 25  | YA    | 444 | C    |
| 25  | YA    | 448 | U    |
| 25  | YA    | 457 | A    |
| 25  | YA    | 470 | A    |
| 25  | YA    | 479 | A    |
| 25  | YA    | 481 | G    |
| 25  | YA    | 483 | A    |
| 25  | YA    | 503 | A    |
| 25  | YA    | 504 | U    |
| 25  | YA    | 505 | A    |
| 25  | YA    | 509 | C    |
| 25  | YA    | 512 | G    |
| 25  | YA    | 518 | G    |
| 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    | 574 | C    |
| 25  | YA    | 575 | A    |
| 25  | YA    | 586 | A    |
| 25  | YA    | 588 | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 603    | A    |
| 25  | YA    | 607    | U    |
| 25  | YA    | 609    | A    |
| 25  | YA    | 614    | U    |
| 25  | YA    | 615    | G    |
| 25  | YA    | 617    | G    |
| 25  | YA    | 622    | G    |
| 25  | YA    | 624    | C    |
| 25  | YA    | 626    | U    |
| 25  | YA    | 627    | A    |
| 25  | YA    | 629    | G    |
| 25  | YA    | 634    | C    |
| 25  | YA    | 637    | A    |
| 25  | YA    | 638    | G    |
| 25  | YA    | 645    | C    |
| 25  | YA    | 646    | A    |
| 25  | YA    | 647    | G    |
| 25  | YA    | 651    | G    |
| 25  | YA    | 654    | A    |
| 25  | YA    | 654(A) | G    |
| 25  | YA    | 654(B) | C    |
| 25  | YA    | 654(T) | C    |
| 25  | YA    | 654(V) | A    |
| 25  | YA    | 668    | G    |
| 25  | YA    | 669    | G    |
| 25  | YA    | 670    | A    |
| 25  | YA    | 676    | A    |
| 25  | YA    | 686    | G    |
| 25  | YA    | 702    | G    |
| 25  | YA    | 705    | A    |
| 25  | YA    | 708    | C    |
| 25  | YA    | 717    | G    |
| 25  | YA    | 722    | A    |
| 25  | YA    | 730    | C    |
| 25  | YA    | 747    | U    |
| 25  | YA    | 753    | C    |
| 25  | YA    | 764    | A    |
| 25  | YA    | 771    | G    |
| 25  | YA    | 776    | G    |
| 25  | YA    | 782    | A    |
| 25  | YA    | 784    | A    |
| 25  | YA    | 785    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | YA    | 790 | C    |
| 25  | YA    | 791 | 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    | 831 | G    |
| 25  | YA    | 847 | U    |
| 25  | YA    | 856 | C    |
| 25  | YA    | 857 | C    |
| 25  | YA    | 860 | U    |
| 25  | YA    | 865 | C    |
| 25  | YA    | 866 | A    |
| 25  | YA    | 877 | U    |
| 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    | 899 | A    |
| 25  | YA    | 900 | A    |
| 25  | YA    | 901 | A    |
| 25  | YA    | 902 | C    |
| 25  | YA    | 905 | U    |
| 25  | YA    | 907 | U    |
| 25  | YA    | 910 | A    |
| 25  | YA    | 915 | C    |
| 25  | YA    | 917 | A    |
| 25  | YA    | 932 | G    |
| 25  | YA    | 936 | C    |
| 25  | YA    | 938 | G    |
| 25  | YA    | 941 | A    |
| 25  | YA    | 945 | A    |
| 25  | YA    | 946 | G    |
| 25  | YA    | 953 | A    |
| 25  | YA    | 959 | A    |
| 25  | YA    | 961 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 974    | G    |
| 25  | YA    | 974(A) | C    |
| 25  | YA    | 975    | G    |
| 25  | YA    | 980    | A    |
| 25  | YA    | 983    | A    |
| 25  | YA    | 989    | G    |
| 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    | 1016   | G    |
| 25  | YA    | 1022   | G    |
| 25  | YA    | 1023   | U    |
| 25  | YA    | 1024   | G    |
| 25  | YA    | 1025   | G    |
| 25  | YA    | 1026   | U    |
| 25  | YA    | 1027   | A    |
| 25  | YA    | 1033   | U    |
| 25  | YA    | 1045   | A    |
| 25  | YA    | 1046   | A    |
| 25  | YA    | 1047   | G    |
| 25  | YA    | 1050   | A    |
| 25  | YA    | 1054   | A    |
| 25  | YA    | 1055   | G    |
| 25  | YA    | 1059   | G    |
| 25  | YA    | 1060   | U    |
| 25  | YA    | 1061   | U    |
| 25  | YA    | 1066   | U    |
| 25  | YA    | 1067   | A    |
| 25  | YA    | 1068   | G    |
| 25  | YA    | 1071   | G    |
| 25  | YA    | 1076   | C    |
| 25  | YA    | 1077   | A    |
| 25  | YA    | 1078   | U    |
| 25  | YA    | 1079   | C    |
| 25  | YA    | 1082   | U    |
| 25  | YA    | 1083   | U    |
| 25  | YA    | 1084   | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | YA    | 1085    | A    |
| 25  | YA    | 1086    | A    |
| 25  | YA    | 1088    | A    |
| 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    | 1105    | U    |
| 25  | YA    | 1110    | G    |
| 25  | YA    | 1111    | A    |
| 25  | YA    | 1129    | A    |
| 25  | YA    | 1130    | U    |
| 25  | YA    | 1135    | C    |
| 25  | YA    | 1136    | G    |
| 25  | YA    | 1142    | U    |
| 25  | YA    | 1142(A) | A    |
| 25  | YA    | 1151    | G    |
| 25  | YA    | 1170    | G    |
| 25  | YA    | 1173    | G    |
| 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    | 1194    | A    |
| 25  | YA    | 1195    | G    |
| 25  | YA    | 1204    | A    |
| 25  | YA    | 1205    | U    |
| 25  | YA    | 1206    | G    |
| 25  | YA    | 1210    | A    |
| 25  | YA    | 1211    | U    |
| 25  | YA    | 1218    | C    |
| 25  | YA    | 1220    | A    |
| 25  | YA    | 1221    | C    |
| 25  | YA    | 1238    | G    |
| 25  | YA    | 1241    | A    |
| 25  | YA    | 1250    | G    |
| 25  | YA    | 1253    | A    |
| 25  | YA    | 1256    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 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    | 1313    | U    |
| 25  | YA    | 1320    | C    |
| 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    | 1379    | A    |
| 25  | YA    | 1384    | A    |
| 25  | YA    | 1385    | G    |
| 25  | YA    | 1386    | C    |
| 25  | YA    | 1390    | U    |
| 25  | YA    | 1392    | A    |
| 25  | YA    | 1395    | A    |
| 25  | YA    | 1398    | C    |
| 25  | YA    | 1407    | C    |
| 25  | YA    | 1411    | C    |
| 25  | YA    | 1412    | A    |
| 25  | YA    | 1416    | G    |
| 25  | YA    | 1419    | A    |
| 25  | YA    | 1420    | U    |
| 25  | YA    | 1421    | G    |
| 25  | YA    | 1428    | C    |
| 25  | YA    | 1429    | G    |
| 25  | YA    | 1444(A) | A    |
| 25  | YA    | 1445    | C    |
| 25  | YA    | 1449    | A    |
| 25  | YA    | 1449(A) | G    |
| 25  | YA    | 1455    | G    |
| 25  | YA    | 1458    | C    |
| 25  | YA    | 1460    | A    |
| 25  | YA    | 1461    | G    |
| 25  | YA    | 1467    | C    |
| 25  | YA    | 1471    | A    |
| 25  | YA    | 1473    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 1474 | C    |
| 25  | YA    | 1478 | G    |
| 25  | YA    | 1479 | G    |
| 25  | YA    | 1482 | U    |
| 25  | YA    | 1483 | G    |
| 25  | YA    | 1485 | G    |
| 25  | YA    | 1490 | A    |
| 25  | YA    | 1491 | G    |
| 25  | YA    | 1493 | C    |
| 25  | YA    | 1496 | A    |
| 25  | YA    | 1497 | U    |
| 25  | YA    | 1505 | C    |
| 25  | YA    | 1506 | C    |
| 25  | YA    | 1507 | A    |
| 25  | YA    | 1508 | A    |
| 25  | YA    | 1510 | A    |
| 25  | YA    | 1511 | A    |
| 25  | YA    | 1513 | C    |
| 25  | YA    | 1514 | U    |
| 25  | YA    | 1516 | U    |
| 25  | YA    | 1518 | C    |
| 25  | YA    | 1522 | G    |
| 25  | YA    | 1525 | G    |
| 25  | YA    | 1534 | G    |
| 25  | YA    | 1535 | U    |
| 25  | YA    | 1536 | A    |
| 25  | YA    | 1537 | C    |
| 25  | YA    | 1540 | G    |
| 25  | YA    | 1543 | A    |
| 25  | YA    | 1544 | C    |
| 25  | YA    | 1545 | A    |
| 25  | YA    | 1549 | C    |
| 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    | 1581 | G    |
| 25  | YA    | 1585 | C    |
| 25  | YA    | 1586 | A    |
| 25  | YA    | 1598 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 1608 | A    |
| 25  | YA    | 1609 | A    |
| 25  | YA    | 1610 | A    |
| 25  | YA    | 1617 | C    |
| 25  | YA    | 1618 | A    |
| 25  | YA    | 1648 | C    |
| 25  | YA    | 1654 | A    |
| 25  | YA    | 1667 | G    |
| 25  | YA    | 1669 | A    |
| 25  | YA    | 1674 | G    |
| 25  | YA    | 1695 | G    |
| 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    | 1780 | A    |
| 25  | YA    | 1782 | 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    | 1819 | A    |
| 25  | YA    | 1820 | U    |
| 25  | YA    | 1829 | A    |
| 25  | YA    | 1835 | G    |
| 25  | YA    | 1847 | A    |
| 25  | YA    | 1848 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 1858 | G    |
| 25  | YA    | 1869 | G    |
| 25  | YA    | 1870 | C    |
| 25  | YA    | 1872 | A    |
| 25  | YA    | 1878 | G    |
| 25  | YA    | 1882 | C    |
| 25  | YA    | 1884 | A    |
| 25  | YA    | 1888 | G    |
| 25  | YA    | 1889 | A    |
| 25  | YA    | 1896 | G    |
| 25  | YA    | 1906 | G    |
| 25  | YA    | 1913 | A    |
| 25  | YA    | 1930 | G    |
| 25  | YA    | 1931 | U    |
| 25  | YA    | 1936 | A    |
| 25  | YA    | 1937 | A    |
| 25  | YA    | 1938 | A    |
| 25  | YA    | 1939 | U    |
| 25  | YA    | 1955 | U    |
| 25  | YA    | 1963 | U    |
| 25  | YA    | 1964 | G    |
| 25  | YA    | 1966 | A    |
| 25  | YA    | 1967 | C    |
| 25  | YA    | 1969 | A    |
| 25  | YA    | 1970 | A    |
| 25  | YA    | 1971 | A    |
| 25  | YA    | 1972 | A    |
| 25  | YA    | 1982 | C    |
| 25  | YA    | 1991 | U    |
| 25  | YA    | 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    | 2055 | C    |
| 25  | YA    | 2056 | G    |
| 25  | YA    | 2059 | A    |
| 25  | YA    | 2060 | A    |
| 25  | YA    | 2061 | G    |
| 25  | YA    | 2062 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2063 | C    |
| 25  | YA    | 2069 | G    |
| 25  | YA    | 2100 | G    |
| 25  | YA    | 2111 | C    |
| 25  | YA    | 2113 | U    |
| 25  | YA    | 2114 | A    |
| 25  | YA    | 2115 | G    |
| 25  | YA    | 2116 | G    |
| 25  | YA    | 2117 | A    |
| 25  | YA    | 2118 | U    |
| 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    | 2190 | G    |
| 25  | YA    | 2192 | G    |
| 25  | YA    | 2198 | A    |
| 25  | YA    | 2210 | G    |
| 25  | YA    | 2211 | G    |
| 25  | YA    | 2212 | A    |
| 25  | YA    | 2215 | G    |
| 25  | YA    | 2225 | A    |
| 25  | YA    | 2238 | G    |
| 25  | YA    | 2243 | U    |
| 25  | YA    | 2246 | G    |
| 25  | YA    | 2275 | C    |
| 25  | YA    | 2283 | C    |
| 25  | YA    | 2287 | A    |
| 25  | YA    | 2288 | A    |
| 25  | YA    | 2307 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2308 | G    |
| 25  | YA    | 2311 | A    |
| 25  | YA    | 2319 | G    |
| 25  | YA    | 2320 | A    |
| 25  | YA    | 2325 | G    |
| 25  | YA    | 2327 | A    |
| 25  | YA    | 2334 | G    |
| 25  | YA    | 2344 | U    |
| 25  | YA    | 2345 | G    |
| 25  | YA    | 2346 | A    |
| 25  | YA    | 2347 | C    |
| 25  | YA    | 2350 | C    |
| 25  | YA    | 2362 | G    |
| 25  | YA    | 2372 | G    |
| 25  | YA    | 2379 | G    |
| 25  | YA    | 2382 | G    |
| 25  | YA    | 2383 | G    |
| 25  | YA    | 2385 | C    |
| 25  | YA    | 2394 | C    |
| 25  | YA    | 2402 | C    |
| 25  | YA    | 2403 | C    |
| 25  | YA    | 2406 | U    |
| 25  | YA    | 2410 | G    |
| 25  | YA    | 2423 | U    |
| 25  | YA    | 2424 | C    |
| 25  | YA    | 2426 | A    |
| 25  | YA    | 2427 | C    |
| 25  | YA    | 2429 | G    |
| 25  | YA    | 2430 | A    |
| 25  | YA    | 2435 | A    |
| 25  | YA    | 2439 | A    |
| 25  | YA    | 2440 | C    |
| 25  | YA    | 2441 | C    |
| 25  | YA    | 2445 | G    |
| 25  | YA    | 2448 | A    |
| 25  | YA    | 2450 | A    |
| 25  | YA    | 2469 | A    |
| 25  | YA    | 2470 | G    |
| 25  | YA    | 2475 | C    |
| 25  | YA    | 2476 | A    |
| 25  | YA    | 2478 | A    |
| 25  | YA    | 2480 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2494 | G    |
| 25  | YA    | 2498 | C    |
| 25  | YA    | 2502 | G    |
| 25  | YA    | 2505 | G    |
| 25  | YA    | 2506 | U    |
| 25  | YA    | 2507 | C    |
| 25  | YA    | 2518 | A    |
| 25  | YA    | 2524 | G    |
| 25  | YA    | 2525 | G    |
| 25  | YA    | 2529 | G    |
| 25  | YA    | 2542 | A    |
| 25  | YA    | 2543 | G    |
| 25  | YA    | 2549 | G    |
| 25  | YA    | 2554 | U    |
| 25  | YA    | 2567 | G    |
| 25  | YA    | 2569 | G    |
| 25  | YA    | 2573 | C    |
| 25  | YA    | 2582 | G    |
| 25  | YA    | 2585 | U    |
| 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    | 2641 | G    |
| 25  | YA    | 2646 | C    |
| 25  | YA    | 2655 | G    |
| 25  | YA    | 2656 | U    |
| 25  | YA    | 2665 | A    |
| 25  | YA    | 2673 | G    |
| 25  | YA    | 2679 | A    |
| 25  | YA    | 2682 | U    |
| 25  | YA    | 2689 | U    |
| 25  | YA    | 2690 | C    |
| 25  | YA    | 2691 | C    |
| 25  | YA    | 2702 | U    |
| 25  | YA    | 2703 | C    |
| 25  | YA    | 2707 | G    |
| 25  | YA    | 2712 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | YA    | 2712(A) | A    |
| 25  | YA    | 2713    | A    |
| 25  | YA    | 2714    | G    |
| 25  | YA    | 2718    | G    |
| 25  | YA    | 2724    | C    |
| 25  | YA    | 2726    | U    |
| 25  | YA    | 2733    | A    |
| 25  | YA    | 2744    | G    |
| 25  | YA    | 2757    | A    |
| 25  | YA    | 2758    | A    |
| 25  | YA    | 2761    | G    |
| 25  | YA    | 2762    | G    |
| 25  | YA    | 2764    | A    |
| 25  | YA    | 2765    | A    |
| 25  | YA    | 2766    | G    |
| 25  | YA    | 2770    | 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    | 2807    | G    |
| 25  | YA    | 2808    | U    |
| 25  | YA    | 2813    | A    |
| 25  | YA    | 2818    | G    |
| 25  | YA    | 2820    | A    |
| 25  | YA    | 2821    | A    |
| 25  | YA    | 2832    | U    |
| 25  | YA    | 2833    | G    |
| 25  | YA    | 2834    | G    |
| 25  | YA    | 2835    | A    |
| 25  | YA    | 2847    | U    |
| 25  | YA    | 2849    | U    |
| 25  | YA    | 2867    | G    |
| 25  | YA    | 2868    | A    |
| 25  | YA    | 2872    | G    |
| 25  | YA    | 2873    | A    |
| 25  | YA    | 2874    | C    |
| 25  | YA    | 2891    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2892 | A    |
| 25  | YA    | 2894 | G    |
| 26  | YB    | 8    | U    |
| 26  | YB    | 9    | G    |
| 26  | YB    | 13   | A    |
| 26  | YB    | 15   | A    |
| 26  | YB    | 19   | G    |
| 26  | YB    | 21   | G    |
| 26  | YB    | 25   | A    |
| 26  | YB    | 27   | C    |
| 26  | YB    | 33   | G    |
| 26  | YB    | 41   | U    |
| 26  | YB    | 42   | C    |
| 26  | YB    | 44   | G    |
| 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    | 88   | C    |
| 26  | YB    | 89   | G    |
| 26  | YB    | 101  | A    |
| 26  | YB    | 105  | G    |
| 26  | YB    | 109  | G    |

All (223) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 31  | G    |
| 1   | QA    | 64  | G    |
| 1   | QA    | 115 | G    |
| 1   | QA    | 181 | G    |
| 1   | QA    | 190 | G    |
| 1   | QA    | 243 | A    |
| 1   | QA    | 244 | U    |
| 1   | QA    | 250 | A    |
| 1   | QA    | 266 | G    |
| 1   | QA    | 328 | C    |
| 1   | QA    | 352 | C    |
| 1   | QA    | 410 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 412    | A    |
| 1   | QA    | 428    | G    |
| 1   | QA    | 481    | G    |
| 1   | QA    | 484    | G    |
| 1   | QA    | 485    | G    |
| 1   | QA    | 509    | A    |
| 1   | QA    | 533    | A    |
| 1   | QA    | 560    | U    |
| 1   | QA    | 595    | G    |
| 1   | QA    | 687    | A    |
| 1   | QA    | 701    | C    |
| 1   | QA    | 703    | G    |
| 1   | QA    | 753    | A    |
| 1   | QA    | 792    | A    |
| 1   | QA    | 812    | C    |
| 1   | QA    | 913    | A    |
| 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    | 1285   | A    |
| 1   | QA    | 1297   | C    |
| 1   | QA    | 1336   | C    |
| 1   | QA    | 1347   | G    |
| 1   | QA    | 1446   | A    |
| 1   | QA    | 1498   | U    |
| 1   | QA    | 1503   | A    |
| 1   | QA    | 1528   | U    |
| 22  | QV    | 53     | G    |
| 23  | QY    | 30     | C    |
| 24  | QX    | 6      | G    |
| 25  | RA    | 74     | A    |
| 25  | RA    | 99     | U    |
| 25  | RA    | 102    | 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    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 271(C) | U    |
| 25  | RA    | 277    | C    |
| 25  | RA    | 345    | A    |
| 25  | RA    | 372    | G    |
| 25  | RA    | 404    | C    |
| 25  | RA    | 503    | A    |
| 25  | RA    | 508    | G    |
| 25  | RA    | 512    | G    |
| 25  | RA    | 587    | C    |
| 25  | RA    | 637    | A    |
| 25  | RA    | 704    | G    |
| 25  | RA    | 752    | A    |
| 25  | RA    | 774    | A    |
| 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    | 1141   | U    |
| 25  | RA    | 1178   | C    |
| 25  | RA    | 1204   | A    |
| 25  | RA    | 1210   | A    |
| 25  | RA    | 1312   | U    |
| 25  | RA    | 1427   | A    |
| 25  | RA    | 1543   | A    |
| 25  | RA    | 1558   | A    |
| 25  | RA    | 1653   | G    |
| 25  | RA    | 1694   | C    |
| 25  | RA    | 1786   | A    |
| 25  | RA    | 1799   | G    |
| 25  | RA    | 1819   | A    |
| 25  | RA    | 1929   | G    |
| 25  | RA    | 1930   | G    |
| 25  | RA    | 1980   | G    |
| 25  | RA    | 1992   | G    |
| 25  | RA    | 2060   | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 2126 | A    |
| 25  | RA    | 2198 | 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    | 2778 | A    |
| 25  | RA    | 2832 | U    |
| 25  | RA    | 2848 | G    |
| 25  | RA    | 2867 | G    |
| 26  | RB    | 24   | G    |
| 26  | RB    | 66   | A    |
| 1   | XA    | 5    | U    |
| 1   | XA    | 31   | G    |
| 1   | XA    | 60   | A    |
| 1   | XA    | 64   | G    |
| 1   | XA    | 78   | G    |
| 1   | XA    | 89   | U    |
| 1   | XA    | 115  | G    |
| 1   | XA    | 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    | 372  | C    |
| 1   | XA    | 410  | G    |
| 1   | XA    | 412  | A    |
| 1   | XA    | 429  | U    |
| 1   | XA    | 481  | G    |
| 1   | XA    | 484  | G    |
| 1   | XA    | 485  | G    |
| 1   | XA    | 509  | A    |
| 1   | XA    | 530  | G    |
| 1   | XA    | 560  | U    |
| 1   | XA    | 575  | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | XA    | 595    | G    |
| 1   | XA    | 687    | A    |
| 1   | XA    | 701    | C    |
| 1   | XA    | 703    | G    |
| 1   | XA    | 752    | G    |
| 1   | XA    | 753    | A    |
| 1   | XA    | 792    | A    |
| 1   | XA    | 812    | C    |
| 1   | XA    | 815    | A    |
| 1   | XA    | 913    | A    |
| 1   | XA    | 960    | U    |
| 1   | XA    | 992    | U    |
| 1   | XA    | 1027   | C    |
| 1   | XA    | 1065   | U    |
| 1   | XA    | 1094   | G    |
| 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    |
| 23  | XY    | 30     | C    |
| 24  | XX    | 6      | G    |
| 25  | YA    | 74     | A    |
| 25  | YA    | 99     | U    |
| 25  | YA    | 102    | G    |
| 25  | YA    | 196    | A    |
| 25  | YA    | 205    | G    |
| 25  | YA    | 221    | A    |
| 25  | YA    | 222    | A    |
| 25  | YA    | 229    | A    |
| 25  | YA    | 241    | A    |
| 25  | YA    | 242    | G    |
| 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    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 653    | A    |
| 25  | YA    | 669    | G    |
| 25  | YA    | 704    | G    |
| 25  | YA    | 752    | A    |
| 25  | YA    | 846    | C    |
| 25  | YA    | 856    | C    |
| 25  | YA    | 859    | G    |
| 25  | YA    | 974(A) | C    |
| 25  | YA    | 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    | 1178   | C    |
| 25  | YA    | 1210   | A    |
| 25  | YA    | 1427   | A    |
| 25  | YA    | 1460   | A    |
| 25  | YA    | 1543   | 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    | 1992   | G    |
| 25  | YA    | 2126   | A    |
| 25  | YA    | 2405   | G    |
| 25  | YA    | 2439   | A    |
| 25  | YA    | 2566   | A    |
| 25  | YA    | 2610   | C    |
| 25  | YA    | 2655   | G    |
| 25  | YA    | 2681   | C    |
| 25  | YA    | 2689   | U    |
| 25  | YA    | 2712   | U    |
| 25  | YA    | 2756   | U    |
| 25  | YA    | 2776   | A    |
| 25  | YA    | 2832   | U    |
| 25  | YA    | 2867   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | YB    | 66  | A    |

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

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

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | PPU  | Z8    | 76  | 57,56 | 37,40,41     | 2.58 | 8 (21%)  | 47,57,60    | 2.56 | 15 (31%) |
| 23  | 1MG  | QY    | 37  | 23    | 23,26,27     | 2.43 | 4 (17%)  | 33,39,42    | 2.08 | 8 (24%)  |
| 56  | PPU  | Z6    | 76  | 25,56 | 37,40,41     | 2.58 | 8 (21%)  | 47,57,60    | 2.57 | 15 (31%) |
| 23  | 1MG  | XY    | 37  | 23    | 23,26,27     | 2.44 | 4 (17%)  | 33,39,42    | 2.08 | 8 (24%)  |

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   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 56  | PPU  | Z8    | 76  | 57,56 | -       | 2/25/43/44 | 0/4/4/4 |
| 23  | 1MG  | QY    | 37  | 23    | -       | 0/7/25/26  | 0/3/3/3 |
| 56  | PPU  | Z6    | 76  | 25,56 | -       | 2/25/43/44 | 0/4/4/4 |
| 23  | 1MG  | XY    | 37  | 23    | -       | 0/7/25/26  | 0/3/3/3 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 56  | Z8    | 76  | PPU  | O-C   | 9.63 | 1.41        | 1.23     |
| 56  | Z6    | 76  | PPU  | O-C   | 9.60 | 1.41        | 1.23     |
| 23  | QY    | 37  | 1MG  | C2-N2 | 7.61 | 1.47        | 1.34     |
| 23  | XY    | 37  | 1MG  | C2-N2 | 7.59 | 1.47        | 1.34     |
| 23  | XY    | 37  | 1MG  | C4-N3 | 6.55 | 1.49        | 1.34     |
| 23  | QY    | 37  | 1MG  | C4-N3 | 6.48 | 1.49        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 56  | Z6    | 76  | PPU  | C9-N6  | -6.22 | 1.32        | 1.45     |
| 56  | Z8    | 76  | PPU  | C9-N6  | -6.18 | 1.32        | 1.45     |
| 56  | Z6    | 76  | PPU  | C-N3'  | 5.85  | 1.46        | 1.34     |
| 56  | Z8    | 76  | PPU  | C10-N6 | -5.84 | 1.32        | 1.45     |
| 56  | Z8    | 76  | PPU  | C-N3'  | 5.84  | 1.46        | 1.34     |
| 56  | Z6    | 76  | PPU  | C10-N6 | -5.83 | 1.32        | 1.45     |
| 23  | XY    | 37  | 1MG  | C2-N1  | 4.67  | 1.45        | 1.37     |
| 23  | QY    | 37  | 1MG  | C2-N1  | 4.60  | 1.45        | 1.37     |
| 56  | Z6    | 76  | PPU  | C5-N7  | -3.59 | 1.32        | 1.39     |
| 56  | Z8    | 76  | PPU  | C5-N7  | -3.58 | 1.32        | 1.39     |
| 56  | Z8    | 76  | PPU  | C8-N9  | -3.26 | 1.32        | 1.37     |
| 56  | Z6    | 76  | PPU  | C8-N9  | -3.25 | 1.32        | 1.37     |
| 56  | Z6    | 76  | PPU  | C1'-N9 | 2.75  | 1.53        | 1.46     |
| 56  | Z8    | 76  | PPU  | C1'-N9 | 2.73  | 1.53        | 1.46     |
| 23  | XY    | 37  | 1MG  | C5-N7  | -2.47 | 1.34        | 1.39     |
| 23  | QY    | 37  | 1MG  | C5-N7  | -2.44 | 1.34        | 1.39     |
| 56  | Z6    | 76  | PPU  | C4-N9  | -2.17 | 1.33        | 1.37     |
| 56  | Z8    | 76  | PPU  | C4-N9  | -2.10 | 1.33        | 1.37     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 56  | Z8    | 76  | PPU  | C3'-N3'-C  | -8.52 | 110.23      | 123.20   |
| 56  | Z6    | 76  | PPU  | C3'-N3'-C  | -8.50 | 110.27      | 123.20   |
| 23  | QY    | 37  | 1MG  | N2-C2-N1   | 6.79  | 124.25      | 118.79   |
| 23  | XY    | 37  | 1MG  | N2-C2-N1   | 6.71  | 124.18      | 118.79   |
| 56  | Z8    | 76  | PPU  | C2'-C1'-N9 | -5.96 | 98.49       | 113.30   |
| 56  | Z6    | 76  | PPU  | C2'-C1'-N9 | -5.93 | 98.56       | 113.30   |
| 56  | Z6    | 76  | PPU  | C5-C4-N3   | -5.03 | 119.80      | 126.72   |
| 56  | Z8    | 76  | PPU  | C5-C4-N3   | -4.96 | 119.88      | 126.72   |
| 56  | Z8    | 76  | PPU  | N3-C2-N1   | -4.80 | 121.31      | 128.58   |
| 56  | Z6    | 76  | PPU  | N3-C2-N1   | -4.77 | 121.36      | 128.58   |
| 23  | XY    | 37  | 1MG  | C5-C4-N3   | -4.73 | 120.86      | 128.39   |
| 23  | QY    | 37  | 1MG  | C5-C4-N3   | -4.66 | 120.97      | 128.39   |
| 56  | Z6    | 76  | PPU  | CA-C-N3'   | 4.11  | 121.77      | 116.21   |
| 56  | Z6    | 76  | PPU  | C2-N1-C6   | 4.09  | 121.82      | 111.83   |
| 56  | Z6    | 76  | PPU  | C4-C5-N7   | -4.05 | 105.95      | 110.58   |
| 56  | Z8    | 76  | PPU  | CA-C-N3'   | 4.05  | 121.69      | 116.21   |
| 56  | Z8    | 76  | PPU  | C2-N1-C6   | 4.04  | 121.71      | 111.83   |
| 56  | Z8    | 76  | PPU  | C4-C5-N7   | -4.01 | 106.00      | 110.58   |
| 23  | XY    | 37  | 1MG  | C2-N3-C4   | 3.91  | 120.77      | 111.98   |
| 23  | QY    | 37  | 1MG  | C2-N3-C4   | 3.90  | 120.73      | 111.98   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 56  | Z6    | 76  | PPU  | C2-N3-C4   | 3.71  | 120.90      | 111.83   |
| 56  | Z8    | 76  | PPU  | C2-N3-C4   | 3.71  | 120.89      | 111.83   |
| 56  | Z6    | 76  | PPU  | C5-N7-C8   | 3.60  | 109.10      | 103.45   |
| 23  | XY    | 37  | 1MG  | N9-C4-N3   | 3.59  | 133.13      | 125.95   |
| 56  | Z8    | 76  | PPU  | C5-N7-C8   | 3.56  | 109.04      | 103.45   |
| 23  | QY    | 37  | 1MG  | N9-C4-N3   | 3.53  | 133.02      | 125.95   |
| 56  | Z6    | 76  | PPU  | CM-OC-CZ   | -3.46 | 110.07      | 117.50   |
| 23  | QY    | 37  | 1MG  | C2-N1-C6   | 3.43  | 123.85      | 120.99   |
| 56  | Z8    | 76  | PPU  | CM-OC-CZ   | -3.42 | 110.16      | 117.50   |
| 56  | Z6    | 76  | PPU  | N9-C8-N7   | -3.41 | 109.11      | 113.94   |
| 56  | Z8    | 76  | PPU  | N9-C8-N7   | -3.36 | 109.17      | 113.94   |
| 23  | XY    | 37  | 1MG  | C2-N1-C6   | 3.31  | 123.75      | 120.99   |
| 56  | Z6    | 76  | PPU  | O4'-C1'-N9 | -2.99 | 102.34      | 108.09   |
| 56  | Z8    | 76  | PPU  | O4'-C1'-N9 | -2.99 | 102.34      | 108.09   |
| 56  | Z6    | 76  | PPU  | N3-C4-N9   | 2.93  | 132.15      | 127.17   |
| 56  | Z8    | 76  | PPU  | N3-C4-N9   | 2.87  | 132.04      | 127.17   |
| 23  | XY    | 37  | 1MG  | C8-N7-C5   | 2.59  | 108.88      | 104.26   |
| 23  | QY    | 37  | 1MG  | C8-N7-C5   | 2.52  | 108.76      | 104.26   |
| 56  | Z6    | 76  | PPU  | C4-C5-C6   | 2.41  | 118.41      | 115.91   |
| 56  | Z8    | 76  | PPU  | C4-C5-C6   | 2.36  | 118.35      | 115.91   |
| 23  | QY    | 37  | 1MG  | O6-C6-C5   | -2.08 | 119.23      | 124.59   |
| 56  | Z8    | 76  | PPU  | C5-C4-N9   | 2.08  | 108.07      | 105.81   |
| 23  | XY    | 37  | 1MG  | O6-C6-C5   | -2.06 | 119.27      | 124.59   |
| 23  | XY    | 37  | 1MG  | C6-C5-N7   | 2.06  | 133.94      | 129.36   |
| 56  | Z6    | 76  | PPU  | C5-C4-N9   | 2.06  | 108.05      | 105.81   |
| 23  | QY    | 37  | 1MG  | C6-C5-N7   | 2.05  | 133.92      | 129.36   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 56  | Z6    | 76  | PPU  | O-C-CA-N   |
| 56  | Z8    | 76  | PPU  | O-C-CA-N   |
| 56  | Z6    | 76  | PPU  | N3'-C-CA-N |
| 56  | Z8    | 76  | PPU  | N3'-C-CA-N |

There are no ring outliers.

2 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56  | Z8    | 76  | PPU  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56  | Z6    | 76  | PPU  | 6       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 680 ligands modelled in this entry, 678 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    | 1675 | -    | 44,45,45     | 1.32 | 5 (11%)  | 63,67,67    | 1.30 | 4 (6%)   |
| 58  | PAR  | QA    | 1666 | -    | 44,45,45     | 1.27 | 6 (13%)  | 63,67,67    | 1.33 | 8 (12%)  |

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    | 1675 | -    | -       | 6/18/94/94 | 0/4/4/4 |
| 58  | PAR  | QA    | 1666 | -    | -       | 8/18/94/94 | 0/4/4/4 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58  | QA    | 1666 | PAR  | C52-C42 | 3.15 | 1.58        | 1.52     |
| 58  | XA    | 1675 | PAR  | C52-C42 | 2.98 | 1.58        | 1.52     |
| 58  | XA    | 1675 | PAR  | C11-C21 | 2.84 | 1.57        | 1.52     |
| 58  | XA    | 1675 | PAR  | O54-C14 | 2.84 | 1.49        | 1.41     |
| 58  | QA    | 1666 | PAR  | O54-C14 | 2.82 | 1.49        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58  | XA    | 1675 | PAR  | O51-C11 | 2.62 | 1.48        | 1.41     |
| 58  | QA    | 1666 | PAR  | C11-C21 | 2.32 | 1.56        | 1.52     |
| 58  | XA    | 1675 | PAR  | C14-C24 | 2.31 | 1.56        | 1.52     |
| 58  | QA    | 1666 | PAR  | O51-C11 | 2.25 | 1.47        | 1.41     |
| 58  | QA    | 1666 | PAR  | C31-C21 | 2.12 | 1.56        | 1.53     |
| 58  | QA    | 1666 | PAR  | C14-C24 | 2.08 | 1.56        | 1.52     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 58  | XA    | 1675 | PAR  | O33-C14-C24 | 5.00  | 116.27      | 108.08   |
| 58  | XA    | 1675 | PAR  | C14-O54-C54 | 4.34  | 122.20      | 113.72   |
| 58  | QA    | 1666 | PAR  | O33-C14-C24 | 4.05  | 114.70      | 108.08   |
| 58  | QA    | 1666 | PAR  | C14-O54-C54 | 3.82  | 121.18      | 113.72   |
| 58  | QA    | 1666 | PAR  | O11-C42-C52 | 3.15  | 115.42      | 107.42   |
| 58  | QA    | 1666 | PAR  | O11-C42-C32 | -3.11 | 101.77      | 109.18   |
| 58  | QA    | 1666 | PAR  | O54-C54-C64 | 2.85  | 111.54      | 106.07   |
| 58  | XA    | 1675 | PAR  | O54-C54-C64 | 2.74  | 111.33      | 106.07   |
| 58  | XA    | 1675 | PAR  | C11-O51-C51 | 2.59  | 118.77      | 113.72   |
| 58  | QA    | 1666 | PAR  | C22-C32-C42 | 2.15  | 114.77      | 109.50   |
| 58  | QA    | 1666 | PAR  | O54-C54-C44 | -2.15 | 105.83      | 109.70   |
| 58  | QA    | 1666 | PAR  | O41-C41-C51 | 2.02  | 114.31      | 109.32   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

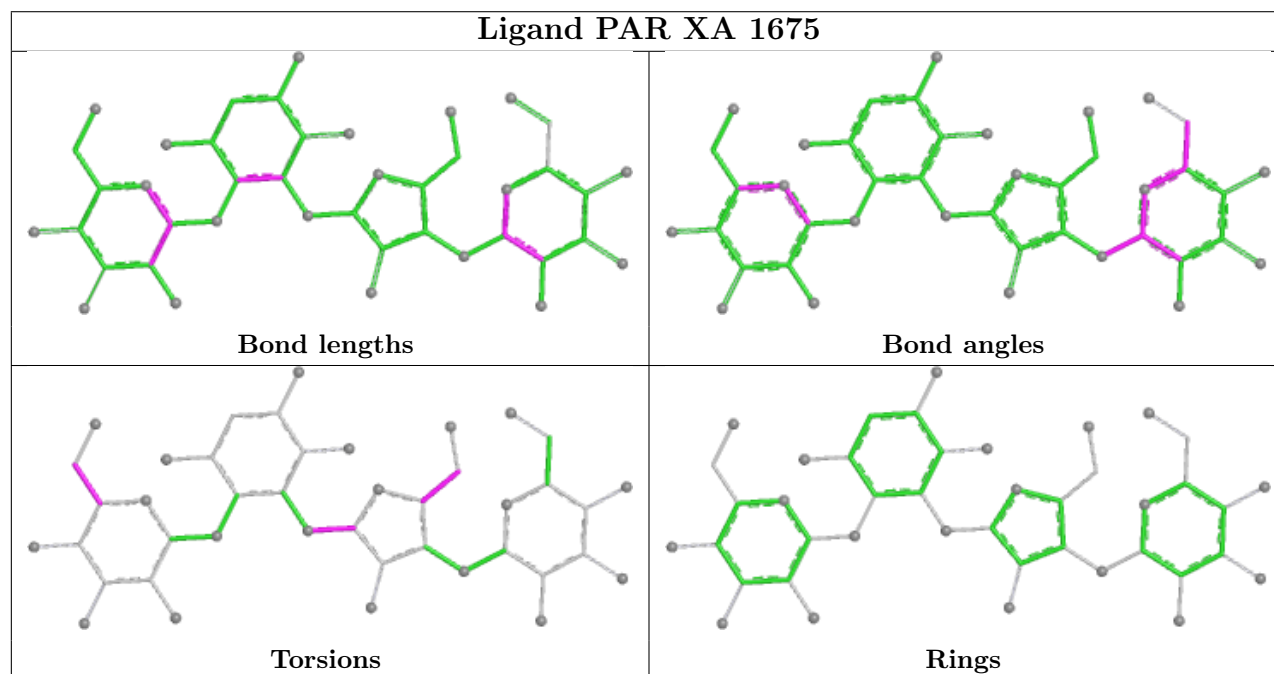
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 58  | QA    | 1666 | PAR  | C44-C54-C64-N64 |
| 58  | QA    | 1666 | PAR  | O54-C54-C64-N64 |
| 58  | XA    | 1675 | PAR  | O51-C51-C61-O61 |
| 58  | QA    | 1666 | PAR  | O51-C51-C61-O61 |
| 58  | XA    | 1675 | PAR  | C41-C51-C61-O61 |
| 58  | QA    | 1666 | PAR  | C41-C51-C61-O61 |
| 58  | XA    | 1675 | PAR  | C33-C43-C53-O53 |
| 58  | XA    | 1675 | PAR  | O43-C43-C53-O53 |
| 58  | QA    | 1666 | PAR  | O43-C13-O52-C52 |
| 58  | XA    | 1675 | PAR  | O43-C13-O52-C52 |
| 58  | QA    | 1666 | PAR  | C23-C13-O52-C52 |
| 58  | XA    | 1675 | PAR  | C23-C13-O52-C52 |
| 58  | QA    | 1666 | PAR  | C23-C33-O33-C14 |
| 58  | QA    | 1666 | PAR  | C43-C33-O33-C14 |

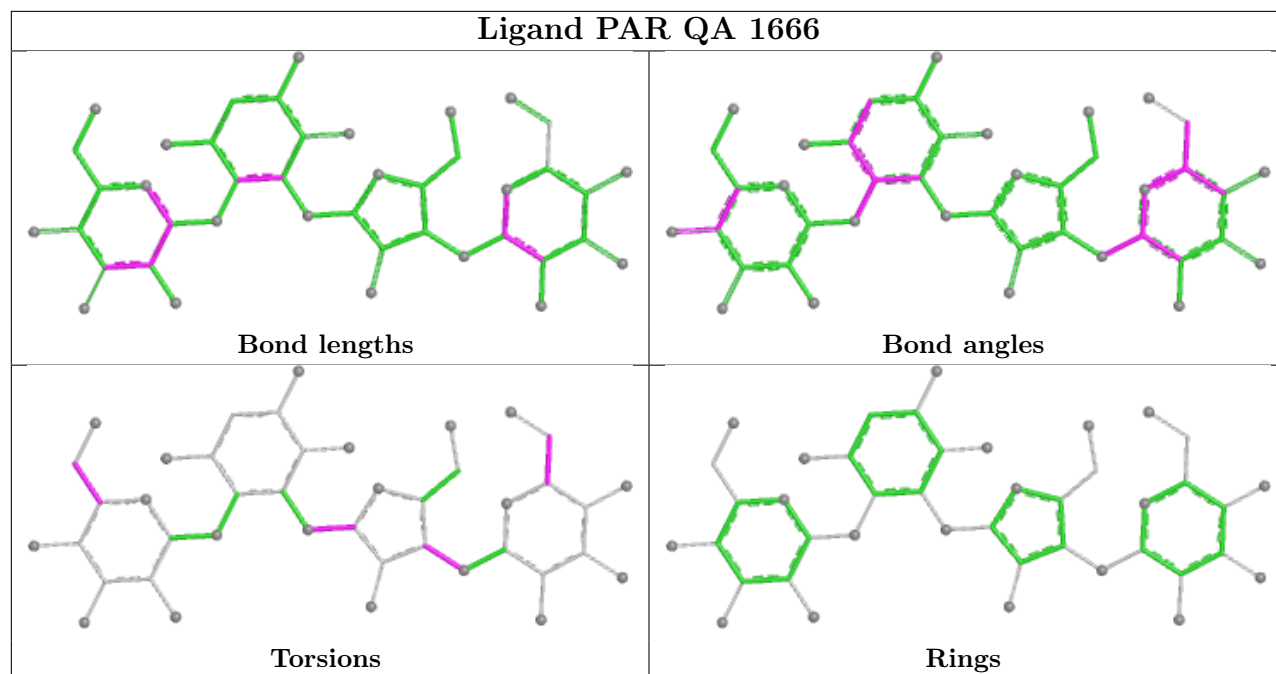
There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | XA    | 1675 | 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%) | 0.55   | 91 (6%) 27 17 | 43, 89, 165, 301      | 0     |
| 1   | XA    | 1500/1522 (98%) | 0.43   | 73 (4%) 35 20 | 33, 76, 161, 285      | 0     |
| 2   | QB    | 237/256 (92%)   | 1.44   | 55 (23%) 2 2  | 74, 140, 206, 264     | 0     |
| 2   | XB    | 237/256 (92%)   | 1.34   | 50 (21%) 2 3  | 68, 121, 186, 246     | 0     |
| 3   | QC    | 205/239 (85%)   | 1.29   | 33 (16%) 4 5  | 66, 125, 179, 210     | 0     |
| 3   | XC    | 205/239 (85%)   | 1.06   | 28 (13%) 6 6  | 46, 95, 150, 198      | 0     |
| 4   | QD    | 208/209 (99%)   | 1.48   | 58 (27%) 1 2  | 47, 92, 146, 223      | 0     |
| 4   | XD    | 208/209 (99%)   | 1.60   | 63 (30%) 1 2  | 45, 96, 162, 182      | 0     |
| 5   | QE    | 151/162 (93%)   | 1.31   | 34 (22%) 2 2  | 42, 101, 170, 220     | 0     |
| 5   | XE    | 151/162 (93%)   | 1.09   | 19 (12%) 8 6  | 35, 84, 142, 186      | 0     |
| 6   | QF    | 101/101 (100%)  | 1.14   | 17 (16%) 4 4  | 40, 90, 127, 156      | 0     |
| 6   | XF    | 101/101 (100%)  | 0.94   | 10 (9%) 13 9  | 38, 84, 127, 150      | 0     |
| 7   | QG    | 155/156 (99%)   | 1.41   | 35 (22%) 2 2  | 56, 121, 175, 232     | 0     |
| 7   | XG    | 155/156 (99%)   | 1.25   | 28 (18%) 3 4  | 51, 93, 148, 196      | 0     |
| 8   | QH    | 138/138 (100%)  | 1.29   | 25 (18%) 3 4  | 51, 100, 142, 160     | 0     |
| 8   | XH    | 138/138 (100%)  | 1.05   | 17 (12%) 8 7  | 51, 89, 134, 187      | 0     |
| 9   | QI    | 127/128 (99%)   | 1.87   | 45 (35%) 1 1  | 71, 131, 189, 204     | 0     |
| 9   | XI    | 127/128 (99%)   | 1.65   | 40 (31%) 1 1  | 46, 112, 165, 221     | 0     |
| 10  | QJ    | 99/105 (94%)    | 2.51   | 56 (56%) 0 0  | 80, 153, 212, 237     | 0     |
| 10  | XJ    | 99/105 (94%)    | 2.03   | 43 (43%) 0 1  | 42, 120, 186, 217     | 0     |
| 11  | QK    | 119/129 (92%)   | 1.57   | 33 (27%) 1 2  | 42, 89, 165, 231      | 0     |
| 11  | XK    | 119/129 (92%)   | 1.15   | 22 (18%) 3 4  | 49, 81, 135, 193      | 0     |
| 12  | QL    | 125/132 (94%)   | 1.41   | 30 (24%) 2 2  | 40, 83, 150, 208      | 0     |
| 12  | XL    | 125/132 (94%)   | 1.16   | 25 (20%) 3 3  | 29, 68, 134, 239      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  | OWAB(Å²) |    | Q<0.9             |   |
|-----|-------|-----------------|--------|----------|----------|----|-------------------|---|
| 13  | QM    | 121/126 (96%)   | 1.82   | 47 (38%) | 1        | 1  | 52, 130, 190, 269 | 0 |
| 13  | XM    | 121/126 (96%)   | 1.63   | 38 (31%) | 1        | 1  | 43, 98, 161, 256  | 0 |
| 14  | QN    | 60/61 (98%)     | 2.23   | 32 (53%) | 0        | 1  | 72, 121, 165, 182 | 0 |
| 14  | XN    | 60/61 (98%)     | 2.01   | 24 (40%) | 1        | 1  | 38, 87, 148, 182  | 0 |
| 15  | QO    | 88/89 (98%)     | 1.27   | 17 (19%) | 3        | 3  | 48, 95, 154, 187  | 0 |
| 15  | XO    | 88/89 (98%)     | 0.94   | 7 (7%)   | 18       | 13 | 43, 82, 128, 167  | 0 |
| 16  | QP    | 84/88 (95%)     | 1.64   | 23 (27%) | 1        | 2  | 44, 86, 146, 195  | 0 |
| 16  | XP    | 84/88 (95%)     | 1.52   | 22 (26%) | 1        | 2  | 46, 92, 133, 208  | 0 |
| 17  | QQ    | 100/105 (95%)   | 1.55   | 31 (31%) | 1        | 1  | 63, 94, 151, 215  | 0 |
| 17  | XQ    | 100/105 (95%)   | 1.48   | 24 (24%) | 2        | 2  | 45, 95, 148, 188  | 0 |
| 18  | QR    | 70/88 (79%)     | 1.03   | 6 (8%)   | 16       | 11 | 45, 85, 146, 166  | 0 |
| 18  | XR    | 70/88 (79%)     | 0.86   | 3 (4%)   | 40       | 22 | 35, 81, 137, 153  | 0 |
| 19  | QS    | 84/93 (90%)     | 1.88   | 34 (40%) | 0        | 1  | 82, 137, 196, 229 | 0 |
| 19  | XS    | 84/93 (90%)     | 1.55   | 23 (27%) | 1        | 2  | 53, 96, 156, 198  | 0 |
| 20  | QT    | 99/106 (93%)    | 1.59   | 31 (31%) | 1        | 1  | 55, 103, 165, 201 | 0 |
| 20  | XT    | 99/106 (93%)    | 1.32   | 24 (24%) | 2        | 2  | 50, 101, 158, 190 | 0 |
| 21  | QU    | 25/27 (92%)     | 3.15   | 19 (76%) | 0        | 0  | 66, 117, 146, 190 | 0 |
| 21  | XU    | 25/27 (92%)     | 2.41   | 13 (52%) | 0        | 1  | 61, 89, 133, 169  | 0 |
| 22  | QV    | 77/77 (100%)    | 1.12   | 6 (7%)   | 19       | 13 | 49, 99, 152, 188  | 0 |
| 22  | XV    | 77/77 (100%)    | 1.01   | 7 (9%)   | 15       | 10 | 43, 82, 137, 198  | 0 |
| 23  | QY    | 14/17 (82%)     | 1.69   | 5 (35%)  | 1        | 1  | 85, 123, 178, 179 | 0 |
| 23  | XY    | 14/17 (82%)     | 1.23   | 2 (14%)  | 6        | 5  | 66, 108, 141, 145 | 0 |
| 24  | QX    | 8/25 (32%)      | 2.78   | 5 (62%)  | 0        | 0  | 68, 91, 144, 227  | 0 |
| 24  | XX    | 8/25 (32%)      | 2.38   | 4 (50%)  | 0        | 1  | 51, 69, 129, 197  | 0 |
| 25  | RA    | 2882/2916 (98%) | 0.36   | 168 (5%) | 29       | 17 | 32, 68, 203, 342  | 0 |
| 25  | YA    | 2883/2916 (98%) | 0.12   | 126 (4%) | 39       | 22 | 21, 52, 190, 313  | 0 |
| 26  | RB    | 120/122 (98%)   | 0.77   | 7 (5%)   | 29       | 17 | 62, 105, 144, 172 | 0 |
| 26  | YB    | 120/122 (98%)   | 0.18   | 2 (1%)   | 69       | 44 | 43, 68, 101, 139  | 0 |
| 27  | RD    | 272/276 (98%)   | 0.99   | 40 (14%) | 6        | 5  | 32, 60, 102, 187  | 0 |
| 27  | YD    | 272/276 (98%)   | 1.17   | 44 (16%) | 4        | 4  | 11, 55, 94, 228   | 0 |
| 28  | RE    | 205/206 (99%)   | 1.36   | 47 (22%) | 2        | 2  | 30, 74, 135, 220  | 0 |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | YE    | 205/206 (99%)  | 0.99   | 30 (14%) 6 5  | 20, 58, 130, 245      | 0     |
| 29  | RF    | 202/210 (96%)  | 1.15   | 33 (16%) 4 4  | 27, 82, 150, 199      | 0     |
| 29  | YF    | 202/210 (96%)  | 0.79   | 19 (9%) 14 10 | 17, 58, 119, 164      | 0     |
| 30  | RG    | 181/182 (99%)  | 3.61   | 142 (78%) 0 0 | 58, 182, 252, 270     | 0     |
| 30  | YG    | 181/182 (99%)  | 2.93   | 125 (69%) 0 0 | 52, 114, 185, 251     | 0     |
| 31  | RH    | 170/180 (94%)  | 1.60   | 55 (32%) 1 1  | 71, 144, 203, 244     | 0     |
| 31  | YH    | 170/180 (94%)  | 1.62   | 53 (31%) 1 1  | 41, 86, 147, 171      | 0     |
| 32  | RI    | 146/148 (98%)  | 0.94   | 19 (13%) 7 6  | 47, 100, 170, 202     | 0     |
| 32  | YI    | 146/148 (98%)  | 0.91   | 17 (11%) 9 7  | 43, 98, 153, 180      | 0     |
| 33  | RN    | 138/140 (98%)  | 1.13   | 18 (13%) 7 6  | 43, 83, 138, 196      | 0     |
| 33  | YN    | 138/140 (98%)  | 1.01   | 21 (15%) 5 5  | 29, 60, 118, 171      | 0     |
| 34  | RO    | 122/122 (100%) | 1.31   | 26 (21%) 2 3  | 21, 75, 123, 179      | 0     |
| 34  | YO    | 122/122 (100%) | 0.60   | 5 (4%) 41 23  | 18, 59, 94, 134       | 0     |
| 35  | RP    | 150/150 (100%) | 1.76   | 49 (32%) 1 1  | 21, 86, 180, 219      | 0     |
| 35  | YP    | 150/150 (100%) | 1.37   | 38 (25%) 1 2  | 14, 67, 136, 235      | 0     |
| 36  | RQ    | 141/141 (100%) | 1.74   | 49 (34%) 1 1  | 45, 88, 145, 231      | 0     |
| 36  | YQ    | 141/141 (100%) | 1.30   | 28 (19%) 3 3  | 24, 65, 135, 196      | 0     |
| 37  | RR    | 118/118 (100%) | 1.09   | 16 (13%) 7 6  | 38, 69, 130, 147      | 0     |
| 37  | YR    | 118/118 (100%) | 0.70   | 5 (4%) 40 23  | 26, 55, 91, 142       | 0     |
| 38  | RS    | 111/112 (99%)  | 1.45   | 31 (27%) 1 2  | 49, 104, 167, 222     | 0     |
| 38  | YS    | 111/112 (99%)  | 0.96   | 15 (13%) 7 6  | 39, 71, 123, 181      | 0     |
| 39  | RT    | 137/146 (93%)  | 1.45   | 36 (26%) 1 2  | 42, 86, 185, 226      | 0     |
| 39  | YT    | 137/146 (93%)  | 0.89   | 19 (13%) 6 5  | 25, 70, 160, 220      | 0     |
| 40  | RU    | 117/118 (99%)  | 1.23   | 21 (17%) 3 4  | 31, 69, 130, 222      | 0     |
| 40  | YU    | 117/118 (99%)  | 1.07   | 18 (15%) 5 5  | 21, 50, 107, 201      | 0     |
| 41  | RV    | 101/101 (100%) | 1.11   | 13 (12%) 7 6  | 44, 92, 155, 249      | 0     |
| 41  | YV    | 101/101 (100%) | 1.33   | 24 (23%) 2 2  | 26, 71, 136, 264      | 0     |
| 42  | RW    | 113/113 (100%) | 0.78   | 9 (7%) 18 13  | 31, 63, 128, 188      | 0     |
| 42  | YW    | 113/113 (100%) | 0.62   | 5 (4%) 39 22  | 17, 54, 114, 186      | 0     |
| 43  | RX    | 92/96 (95%)    | 1.18   | 13 (14%) 6 5  | 41, 78, 122, 150      | 0     |
| 43  | YX    | 92/96 (95%)    | 0.87   | 9 (9%) 13 9   | 28, 56, 92, 122       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | RY    | 102/110 (92%)     | 2.29   | 56 (54%) 0 0   | 50, 106, 193, 237     | 0     |
| 44  | YY    | 102/110 (92%)     | 1.57   | 33 (32%) 1 1   | 39, 82, 158, 234      | 0     |
| 45  | RZ    | 183/206 (88%)     | 1.59   | 62 (33%) 1 1   | 56, 124, 189, 247     | 0     |
| 45  | YZ    | 183/206 (88%)     | 1.08   | 31 (16%) 4 4   | 41, 86, 169, 257      | 0     |
| 46  | R0    | 82/85 (96%)       | 0.69   | 5 (6%) 27 17   | 42, 72, 103, 131      | 0     |
| 46  | Y0    | 82/85 (96%)       | 0.29   | 2 (2%) 59 36   | 26, 49, 80, 99        | 0     |
| 47  | R1    | 97/98 (98%)       | 1.74   | 29 (29%) 1 2   | 34, 75, 194, 262      | 0     |
| 47  | Y1    | 97/98 (98%)       | 1.20   | 19 (19%) 3 3   | 27, 61, 143, 210      | 0     |
| 48  | R2    | 69/72 (95%)       | 1.19   | 10 (14%) 6 5   | 48, 94, 168, 184      | 0     |
| 48  | Y2    | 69/72 (95%)       | 1.21   | 14 (20%) 3 3   | 22, 66, 131, 195      | 0     |
| 49  | R3    | 59/60 (98%)       | 1.43   | 14 (23%) 2 2   | 42, 90, 161, 183      | 0     |
| 49  | Y3    | 59/60 (98%)       | 0.66   | 3 (5%) 33 19   | 33, 61, 113, 179      | 0     |
| 50  | R4    | 71/71 (100%)      | 2.33   | 39 (54%) 0 0   | 129, 204, 273, 302    | 0     |
| 50  | Y4    | 71/71 (100%)      | 2.65   | 47 (66%) 0 0   | 84, 166, 258, 313     | 0     |
| 51  | R5    | 59/60 (98%)       | 1.87   | 20 (33%) 1 1   | 25, 73, 191, 257      | 0     |
| 51  | Y5    | 59/60 (98%)       | 1.71   | 22 (37%) 1 1   | 28, 62, 189, 319      | 0     |
| 52  | R6    | 49/54 (90%)       | 3.29   | 34 (69%) 0 0   | 66, 147, 198, 224     | 0     |
| 52  | Y6    | 49/54 (90%)       | 3.19   | 36 (73%) 0 0   | 59, 116, 196, 225     | 0     |
| 53  | R7    | 49/49 (100%)      | 1.49   | 12 (24%) 2 2   | 27, 55, 129, 235      | 0     |
| 53  | Y7    | 49/49 (100%)      | 0.95   | 6 (12%) 8 7    | 23, 42, 102, 186      | 0     |
| 54  | R8    | 64/65 (98%)       | 1.95   | 25 (39%) 1 1   | 34, 73, 129, 210      | 0     |
| 54  | Y8    | 64/65 (98%)       | 1.46   | 12 (18%) 3 3   | 24, 56, 101, 237      | 0     |
| 55  | R9    | 37/37 (100%)      | 2.36   | 16 (43%) 0 1   | 64, 96, 157, 235      | 0     |
| 55  | Y9    | 37/37 (100%)      | 2.52   | 24 (64%) 0 0   | 48, 83, 136, 176      | 0     |
| 56  | Z6    | 2/3 (66%)         | 3.37   | 2 (100%) 0 0   | 77, 77, 77, 77        | 0     |
| 56  | Z8    | 2/3 (66%)         | 3.50   | 2 (100%) 0 0   | 51, 51, 51, 60        | 0     |
| All | All   | 20873/21492 (97%) | 0.94   | 3347 (16%) 5 5 | 11, 79, 179, 342      | 0     |

All (3347) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 50  | Y4    | 66  | SER  | 12.0 |
| 52  | R6    | 42  | TRP  | 11.9 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | Y6    | 42   | TRP  | 11.6 |
| 14  | XN    | 2    | ALA  | 11.0 |
| 52  | R6    | 23   | THR  | 10.5 |
| 50  | Y4    | 67   | TYR  | 9.7  |
| 30  | RG    | 155  | MET  | 9.6  |
| 30  | RG    | 64   | THR  | 9.5  |
| 35  | RP    | 13   | ASN  | 9.3  |
| 51  | R5    | 54   | GLY  | 9.0  |
| 44  | RY    | 58   | GLY  | 8.7  |
| 7   | QG    | 81   | GLY  | 8.7  |
| 14  | XN    | 41   | ARG  | 8.6  |
| 35  | YP    | 13   | ASN  | 8.5  |
| 52  | Y6    | 23   | THR  | 8.5  |
| 11  | QK    | 129  | SER  | 8.5  |
| 25  | YA    | 1536 | A    | 8.5  |
| 36  | RQ    | 140  | ALA  | 8.4  |
| 53  | R7    | 49   | ARG  | 8.3  |
| 8   | QH    | 1    | MET  | 8.2  |
| 30  | YG    | 2    | PRO  | 8.2  |
| 25  | RA    | 1536 | A    | 8.2  |
| 30  | RG    | 72   | ARG  | 8.1  |
| 30  | RG    | 157  | ILE  | 8.0  |
| 53  | Y7    | 48   | LYS  | 8.0  |
| 53  | R7    | 48   | LYS  | 7.9  |
| 36  | YQ    | 80   | GLU  | 7.8  |
| 7   | QG    | 82   | GLY  | 7.8  |
| 40  | YU    | 117  | GLN  | 7.7  |
| 31  | YH    | 3    | ARG  | 7.6  |
| 30  | RG    | 39   | ILE  | 7.6  |
| 19  | XS    | 11   | VAL  | 7.4  |
| 25  | RA    | 1060 | U    | 7.4  |
| 30  | RG    | 93   | THR  | 7.4  |
| 30  | YG    | 93   | THR  | 7.4  |
| 10  | QJ    | 85   | LEU  | 7.3  |
| 55  | Y9    | 21   | GLY  | 7.3  |
| 51  | R5    | 52   | TYR  | 7.3  |
| 17  | XQ    | 99   | SER  | 7.3  |
| 30  | RG    | 65   | GLY  | 7.2  |
| 10  | XJ    | 59   | SER  | 7.2  |
| 17  | QQ    | 101  | ARG  | 7.2  |
| 30  | RG    | 99   | MET  | 7.2  |
| 21  | QU    | 26   | LYS  | 7.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | RG    | 143  | GLU  | 7.1  |
| 39  | RT    | 115  | ARG  | 7.1  |
| 47  | R1    | 95   | LEU  | 7.1  |
| 10  | QJ    | 4    | ILE  | 7.1  |
| 4   | QD    | 2    | GLY  | 7.0  |
| 4   | QD    | 32   | ALA  | 6.9  |
| 27  | RD    | 33   | LEU  | 6.9  |
| 48  | R2    | 8    | LYS  | 6.9  |
| 9   | QI    | 124  | GLN  | 6.9  |
| 14  | QN    | 2    | ALA  | 6.9  |
| 19  | QS    | 75   | ALA  | 6.9  |
| 8   | XH    | 1    | MET  | 6.9  |
| 52  | Y6    | 43   | CYS  | 6.9  |
| 36  | YQ    | 87   | LYS  | 6.8  |
| 7   | XG    | 5    | ARG  | 6.8  |
| 55  | R9    | 1    | MET  | 6.8  |
| 52  | R6    | 40   | CYS  | 6.8  |
| 17  | XQ    | 101  | ARG  | 6.7  |
| 36  | RQ    | 91   | GLU  | 6.7  |
| 52  | R6    | 24   | GLU  | 6.7  |
| 30  | YG    | 116  | ASP  | 6.7  |
| 13  | QM    | 6    | GLY  | 6.7  |
| 30  | YG    | 84   | LYS  | 6.7  |
| 24  | XX    | 8    | A    | 6.6  |
| 25  | RA    | 1058 | G    | 6.6  |
| 9   | QI    | 110  | GLU  | 6.6  |
| 9   | QI    | 117  | HIS  | 6.6  |
| 40  | RU    | 117  | GLN  | 6.6  |
| 30  | RG    | 24   | GLY  | 6.5  |
| 30  | RG    | 68   | PRO  | 6.5  |
| 28  | RE    | 204  | ALA  | 6.5  |
| 30  | RG    | 100  | TRP  | 6.5  |
| 7   | XG    | 84   | ASN  | 6.4  |
| 30  | RG    | 96   | ARG  | 6.4  |
| 30  | RG    | 172  | LEU  | 6.4  |
| 36  | RQ    | 80   | GLU  | 6.4  |
| 30  | RG    | 28   | VAL  | 6.4  |
| 52  | R6    | 5    | VAL  | 6.4  |
| 16  | QP    | 68   | ASP  | 6.3  |
| 21  | QU    | 2    | GLY  | 6.3  |
| 19  | QS    | 11   | VAL  | 6.3  |
| 7   | XG    | 32   | ARG  | 6.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | XU    | 10   | ARG  | 6.3  |
| 1   | QA    | 82   | U    | 6.3  |
| 25  | YA    | 1060 | U    | 6.3  |
| 40  | YU    | 75   | ASN  | 6.2  |
| 30  | RG    | 34   | LEU  | 6.2  |
| 41  | YV    | 45   | THR  | 6.2  |
| 25  | RA    | 2174 | C    | 6.2  |
| 50  | Y4    | 68   | ARG  | 6.2  |
| 54  | R8    | 35   | GLN  | 6.1  |
| 7   | XG    | 85   | TYR  | 6.1  |
| 35  | RP    | 91   | PHE  | 6.1  |
| 50  | R4    | 49   | PHE  | 6.1  |
| 30  | RG    | 58   | GLN  | 6.1  |
| 11  | QK    | 128  | ALA  | 6.1  |
| 13  | QM    | 101  | GLN  | 6.0  |
| 51  | R5    | 50   | GLY  | 6.0  |
| 55  | Y9    | 1    | MET  | 6.0  |
| 36  | RQ    | 21   | THR  | 6.0  |
| 41  | YV    | 36   | PRO  | 6.0  |
| 44  | RY    | 22   | GLY  | 6.0  |
| 9   | XI    | 66   | ARG  | 5.9  |
| 7   | QG    | 37   | ASN  | 5.9  |
| 25  | RA    | 1070 | A    | 5.9  |
| 44  | RY    | 102  | CYS  | 5.9  |
| 30  | RG    | 102  | PHE  | 5.9  |
| 52  | R6    | 46   | HIS  | 5.9  |
| 10  | QJ    | 12   | ASP  | 5.8  |
| 30  | YG    | 135  | LEU  | 5.8  |
| 27  | YD    | 235  | GLY  | 5.8  |
| 44  | RY    | 45   | VAL  | 5.8  |
| 30  | RG    | 33   | ARG  | 5.8  |
| 30  | RG    | 101  | ILE  | 5.8  |
| 44  | RY    | 88   | LYS  | 5.8  |
| 30  | YG    | 155  | MET  | 5.7  |
| 44  | RY    | 89   | PHE  | 5.7  |
| 54  | R8    | 65   | GLU  | 5.7  |
| 50  | R4    | 66   | SER  | 5.7  |
| 47  | R1    | 98   | LEU  | 5.7  |
| 28  | RE    | 193  | GLY  | 5.7  |
| 44  | YY    | 91   | GLU  | 5.7  |
| 11  | XK    | 129  | SER  | 5.7  |
| 35  | RP    | 18   | ARG  | 5.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | RG    | 66   | GLN  | 5.7  |
| 13  | QM    | 100  | GLY  | 5.7  |
| 17  | QQ    | 100  | LYS  | 5.7  |
| 13  | QM    | 7    | VAL  | 5.7  |
| 30  | RG    | 131  | TYR  | 5.6  |
| 17  | XQ    | 97   | SER  | 5.6  |
| 13  | QM    | 122  | LYS  | 5.6  |
| 25  | YA    | 1061 | U    | 5.6  |
| 30  | RG    | 63   | ILE  | 5.6  |
| 4   | XD    | 209  | ARG  | 5.6  |
| 51  | R5    | 45   | VAL  | 5.5  |
| 28  | RE    | 63   | LEU  | 5.5  |
| 45  | YZ    | 121  | HIS  | 5.5  |
| 4   | QD    | 80   | GLU  | 5.5  |
| 13  | XM    | 7    | VAL  | 5.5  |
| 30  | RG    | 92   | VAL  | 5.5  |
| 30  | RG    | 94   | LEU  | 5.5  |
| 30  | RG    | 103  | LEU  | 5.5  |
| 20  | QT    | 9    | ASN  | 5.5  |
| 39  | YT    | 106  | SER  | 5.5  |
| 12  | QL    | 91   | LYS  | 5.5  |
| 4   | XD    | 181  | MET  | 5.5  |
| 5   | XE    | 83   | GLU  | 5.5  |
| 30  | RG    | 60   | LEU  | 5.4  |
| 30  | YG    | 34   | LEU  | 5.4  |
| 19  | QS    | 12   | ASP  | 5.4  |
| 21  | QU    | 16   | GLY  | 5.4  |
| 51  | Y5    | 54   | GLY  | 5.4  |
| 30  | YG    | 157  | ILE  | 5.4  |
| 37  | RR    | 102  | GLU  | 5.4  |
| 30  | YG    | 26   | GLN  | 5.4  |
| 30  | RG    | 142  | PRO  | 5.4  |
| 31  | YH    | 154  | PRO  | 5.4  |
| 10  | QJ    | 45   | ARG  | 5.4  |
| 3   | QC    | 193  | TYR  | 5.4  |
| 24  | QX    | 8    | A    | 5.4  |
| 55  | Y9    | 37   | GLY  | 5.4  |
| 2   | XB    | 217  | ARG  | 5.4  |
| 54  | Y8    | 64   | TYR  | 5.4  |
| 30  | RG    | 95   | ARG  | 5.4  |
| 30  | YG    | 72   | ARG  | 5.4  |
| 53  | Y7    | 49   | ARG  | 5.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | QJ    | 59   | SER  | 5.3  |
| 50  | R4    | 67   | TYR  | 5.3  |
| 30  | RG    | 80   | PHE  | 5.3  |
| 48  | R2    | 52   | ASP  | 5.3  |
| 31  | YH    | 2    | SER  | 5.3  |
| 30  | RG    | 69   | ALA  | 5.3  |
| 9   | QI    | 62   | TYR  | 5.3  |
| 25  | RA    | 1059 | G    | 5.3  |
| 25  | RA    | 1061 | U    | 5.3  |
| 9   | XI    | 7    | THR  | 5.3  |
| 35  | YP    | 109  | GLY  | 5.3  |
| 47  | Y1    | 95   | LEU  | 5.3  |
| 17  | XQ    | 100  | LYS  | 5.3  |
| 30  | RG    | 154  | GLY  | 5.3  |
| 30  | RG    | 111  | LEU  | 5.3  |
| 25  | YA    | 2117 | A    | 5.3  |
| 21  | QU    | 9    | ARG  | 5.3  |
| 13  | XM    | 85   | GLY  | 5.2  |
| 10  | QJ    | 5    | ARG  | 5.2  |
| 30  | RG    | 35   | GLU  | 5.2  |
| 39  | RT    | 1    | MET  | 5.2  |
| 44  | YY    | 81   | LYS  | 5.2  |
| 54  | R8    | 63   | PRO  | 5.2  |
| 2   | QB    | 165  | VAL  | 5.2  |
| 30  | YG    | 172  | LEU  | 5.2  |
| 33  | RN    | 138  | LEU  | 5.2  |
| 21  | QU    | 10   | ARG  | 5.2  |
| 55  | R9    | 37   | GLY  | 5.2  |
| 30  | RG    | 159  | VAL  | 5.2  |
| 54  | Y8    | 35   | GLN  | 5.2  |
| 25  | YA    | 2125 | G    | 5.2  |
| 4   | XD    | 132  | ARG  | 5.2  |
| 13  | XM    | 122  | LYS  | 5.2  |
| 10  | QJ    | 42   | THR  | 5.2  |
| 30  | YG    | 24   | GLY  | 5.1  |
| 9   | XI    | 17   | VAL  | 5.1  |
| 30  | RG    | 87   | PRO  | 5.1  |
| 25  | RA    | 11   | G    | 5.1  |
| 9   | XI    | 110  | GLU  | 5.1  |
| 17  | QQ    | 99   | SER  | 5.1  |
| 10  | QJ    | 43   | ARG  | 5.1  |
| 3   | QC    | 171  | GLY  | 5.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 54  | R8    | 64   | TYR  | 5.1  |
| 7   | QG    | 32   | ARG  | 5.1  |
| 54  | Y8    | 65   | GLU  | 5.1  |
| 31  | YH    | 155  | SER  | 5.1  |
| 25  | RA    | 2116 | G    | 5.1  |
| 9   | QI    | 8    | GLY  | 5.1  |
| 29  | YF    | 207  | GLY  | 5.1  |
| 44  | RY    | 49   | VAL  | 5.1  |
| 55  | R9    | 20   | HIS  | 5.1  |
| 21  | XU    | 26   | LYS  | 5.1  |
| 36  | RQ    | 59   | ARG  | 5.1  |
| 46  | R0    | 2    | ALA  | 5.1  |
| 30  | YG    | 31   | VAL  | 5.1  |
| 52  | R6    | 13   | CYS  | 5.1  |
| 51  | Y5    | 52   | TYR  | 5.1  |
| 30  | RG    | 97   | ASP  | 5.1  |
| 9   | QI    | 127  | LYS  | 5.1  |
| 11  | QK    | 51   | LYS  | 5.1  |
| 30  | YG    | 96   | ARG  | 5.1  |
| 19  | QS    | 5    | LEU  | 5.1  |
| 54  | R8    | 34   | TRP  | 5.0  |
| 1   | XA    | 631  | G    | 5.0  |
| 35  | RP    | 118  | GLY  | 5.0  |
| 21  | QU    | 8    | THR  | 5.0  |
| 30  | YG    | 30   | GLU  | 5.0  |
| 23  | QY    | 32   | U    | 5.0  |
| 2   | XB    | 133  | LYS  | 5.0  |
| 53  | R7    | 23   | ARG  | 5.0  |
| 1   | QA    | 1124 | G    | 5.0  |
| 50  | Y4    | 1    | MET  | 5.0  |
| 30  | RG    | 62   | LEU  | 5.0  |
| 35  | RP    | 114  | ILE  | 5.0  |
| 30  | RG    | 117  | PHE  | 5.0  |
| 35  | RP    | 74   | GLU  | 5.0  |
| 27  | YD    | 38   | LYS  | 5.0  |
| 32  | RI    | 9    | LEU  | 5.0  |
| 35  | RP    | 109  | GLY  | 5.0  |
| 30  | YG    | 20   | ILE  | 4.9  |
| 14  | QN    | 29   | ARG  | 4.9  |
| 30  | RG    | 118  | ARG  | 4.9  |
| 44  | RY    | 81   | LYS  | 4.9  |
| 55  | R9    | 9    | ARG  | 4.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | R1    | 93   | GLU  | 4.9  |
| 30  | RG    | 90   | LEU  | 4.9  |
| 50  | Y4    | 70   | GLY  | 4.9  |
| 10  | XJ    | 5    | ARG  | 4.9  |
| 10  | XJ    | 8    | LEU  | 4.9  |
| 24  | QX    | 7    | G    | 4.9  |
| 7   | XG    | 34   | GLY  | 4.9  |
| 30  | RG    | 29   | TRP  | 4.9  |
| 51  | Y5    | 53   | ALA  | 4.9  |
| 55  | Y9    | 15   | LYS  | 4.9  |
| 42  | RW    | 77   | ASP  | 4.9  |
| 36  | YQ    | 141  | GLN  | 4.9  |
| 47  | Y1    | 48   | LYS  | 4.9  |
| 19  | QS    | 67   | VAL  | 4.9  |
| 1   | QA    | 1182 | G    | 4.9  |
| 13  | XM    | 8    | GLU  | 4.8  |
| 4   | XD    | 3    | ARG  | 4.8  |
| 9   | XI    | 106  | ALA  | 4.8  |
| 11  | QK    | 117  | ASN  | 4.8  |
| 9   | XI    | 105  | ASP  | 4.8  |
| 15  | XO    | 88   | ARG  | 4.8  |
| 30  | YG    | 79   | ASN  | 4.8  |
| 52  | R6    | 11   | LEU  | 4.8  |
| 54  | Y8    | 61   | LEU  | 4.8  |
| 16  | QP    | 72   | ARG  | 4.8  |
| 30  | RG    | 85   | GLY  | 4.8  |
| 36  | YQ    | 140  | ALA  | 4.8  |
| 50  | Y4    | 37   | SER  | 4.8  |
| 30  | YG    | 101  | ILE  | 4.8  |
| 9   | XI    | 64   | THR  | 4.8  |
| 51  | Y5    | 57   | VAL  | 4.8  |
| 44  | YY    | 102  | CYS  | 4.8  |
| 7   | QG    | 83   | ALA  | 4.8  |
| 30  | RG    | 41   | GLN  | 4.8  |
| 30  | YG    | 100  | TRP  | 4.8  |
| 25  | YA    | 2121 | G    | 4.8  |
| 45  | RZ    | 148  | ASP  | 4.8  |
| 30  | YG    | 64   | THR  | 4.8  |
| 31  | RH    | 89   | ILE  | 4.7  |
| 3   | XC    | 2    | GLY  | 4.7  |
| 10  | QJ    | 10   | GLY  | 4.7  |
| 51  | Y5    | 50   | GLY  | 4.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | R6    | 43   | CYS  | 4.7  |
| 50  | R4    | 37   | SER  | 4.7  |
| 50  | Y4    | 26   | SER  | 4.7  |
| 30  | YG    | 178  | PHE  | 4.7  |
| 35  | YP    | 74   | GLU  | 4.7  |
| 2   | XB    | 96   | ARG  | 4.7  |
| 30  | RG    | 141  | PHE  | 4.7  |
| 21  | XU    | 15   | ARG  | 4.7  |
| 1   | XA    | 1182 | G    | 4.7  |
| 28  | YE    | 63   | LEU  | 4.7  |
| 52  | R6    | 22   | ALA  | 4.7  |
| 32  | RI    | 15   | VAL  | 4.7  |
| 54  | R8    | 41   | ILE  | 4.7  |
| 4   | QD    | 84   | LYS  | 4.7  |
| 7   | XG    | 33   | ASP  | 4.6  |
| 10  | QJ    | 73   | ASP  | 4.6  |
| 16  | XP    | 68   | ASP  | 4.6  |
| 29  | RF    | 96   | ASP  | 4.6  |
| 30  | RG    | 148  | MET  | 4.6  |
| 15  | XO    | 3    | ILE  | 4.6  |
| 30  | RG    | 71   | THR  | 4.6  |
| 12  | XL    | 19   | ARG  | 4.6  |
| 39  | RT    | 3    | ARG  | 4.6  |
| 47  | R1    | 80   | LEU  | 4.6  |
| 30  | RG    | 156  | ASP  | 4.6  |
| 48  | Y2    | 70   | GLN  | 4.6  |
| 30  | RG    | 133  | LEU  | 4.6  |
| 1   | QA    | 631  | G    | 4.6  |
| 25  | RA    | 2801 | A    | 4.6  |
| 29  | YF    | 132  | VAL  | 4.6  |
| 30  | YG    | 126  | ASP  | 4.6  |
| 54  | Y8    | 63   | PRO  | 4.6  |
| 30  | RG    | 26   | GLN  | 4.6  |
| 30  | YG    | 53   | LEU  | 4.6  |
| 27  | YD    | 40   | THR  | 4.6  |
| 45  | YZ    | 113  | ALA  | 4.6  |
| 30  | YG    | 74   | LYS  | 4.6  |
| 25  | RA    | 1053 | C    | 4.6  |
| 25  | YA    | 11   | G    | 4.6  |
| 4   | XD    | 154  | ASN  | 4.6  |
| 13  | QM    | 106  | ASN  | 4.6  |
| 27  | RD    | 40   | THR  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | QD    | 31   | CYS  | 4.5  |
| 51  | Y5    | 46   | CYS  | 4.5  |
| 12  | QL    | 19   | ARG  | 4.5  |
| 30  | RG    | 77   | ILE  | 4.5  |
| 35  | YP    | 122  | PRO  | 4.5  |
| 17  | QQ    | 96   | GLU  | 4.5  |
| 39  | RT    | 6    | LEU  | 4.5  |
| 12  | QL    | 95   | GLY  | 4.5  |
| 24  | XX    | 7    | G    | 4.5  |
| 3   | QC    | 160  | ALA  | 4.5  |
| 30  | RG    | 84   | LYS  | 4.5  |
| 9   | QI    | 128  | ARG  | 4.5  |
| 27  | YD    | 33   | LEU  | 4.5  |
| 50  | Y4    | 65   | ASP  | 4.5  |
| 52  | Y6    | 24   | GLU  | 4.5  |
| 25  | RA    | 1057 | A    | 4.5  |
| 25  | RA    | 1064 | C    | 4.5  |
| 25  | YA    | 2402 | C    | 4.5  |
| 10  | QJ    | 98   | ILE  | 4.5  |
| 52  | Y6    | 39   | TYR  | 4.5  |
| 30  | RG    | 53   | LEU  | 4.5  |
| 50  | Y4    | 18   | CYS  | 4.5  |
| 2   | QB    | 160  | ASP  | 4.5  |
| 30  | YG    | 97   | ASP  | 4.5  |
| 10  | XJ    | 47   | PHE  | 4.5  |
| 30  | YG    | 69   | ALA  | 4.5  |
| 16  | XP    | 13   | HIS  | 4.5  |
| 20  | XT    | 73   | HIS  | 4.5  |
| 30  | YG    | 63   | ILE  | 4.5  |
| 35  | RP    | 88   | LEU  | 4.5  |
| 25  | RA    | 2135 | A    | 4.5  |
| 44  | RY    | 82   | PRO  | 4.5  |
| 30  | RG    | 8    | LYS  | 4.5  |
| 30  | RG    | 153  | ARG  | 4.5  |
| 36  | YQ    | 10   | ARG  | 4.5  |
| 22  | XV    | 47   | U    | 4.5  |
| 9   | QI    | 85   | LEU  | 4.5  |
| 30  | YG    | 54   | GLU  | 4.5  |
| 10  | QJ    | 54   | PHE  | 4.5  |
| 36  | YQ    | 24   | GLY  | 4.4  |
| 20  | QT    | 70   | SER  | 4.4  |
| 39  | RT    | 106  | SER  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | R6    | 47   | THR  | 4.4  |
| 4   | XD    | 22   | LYS  | 4.4  |
| 50  | R4    | 69   | LYS  | 4.4  |
| 52  | Y6    | 45   | LYS  | 4.4  |
| 30  | YG    | 92   | VAL  | 4.4  |
| 47  | R1    | 89   | GLU  | 4.4  |
| 50  | R4    | 1    | MET  | 4.4  |
| 13  | QM    | 4    | ILE  | 4.4  |
| 45  | RZ    | 183  | LEU  | 4.4  |
| 38  | YS    | 20   | ARG  | 4.4  |
| 52  | Y6    | 12   | GLU  | 4.4  |
| 30  | RG    | 127  | GLY  | 4.4  |
| 30  | RG    | 88   | ILE  | 4.4  |
| 34  | RO    | 81   | ASP  | 4.4  |
| 9   | QI    | 27   | THR  | 4.4  |
| 30  | RG    | 36   | LYS  | 4.4  |
| 36  | RQ    | 22   | LYS  | 4.4  |
| 52  | Y6    | 47   | THR  | 4.4  |
| 25  | RA    | 2175 | C    | 4.4  |
| 2   | QB    | 163  | PHE  | 4.4  |
| 20  | XT    | 12   | ALA  | 4.4  |
| 30  | YG    | 138  | GLN  | 4.4  |
| 36  | RQ    | 141  | GLN  | 4.4  |
| 28  | RE    | 78   | LEU  | 4.4  |
| 13  | QM    | 120  | LYS  | 4.4  |
| 52  | Y6    | 46   | HIS  | 4.4  |
| 25  | RA    | 2893 | G    | 4.4  |
| 30  | RG    | 132  | ASN  | 4.4  |
| 44  | RY    | 91   | GLU  | 4.4  |
| 5   | QE    | 20   | GLN  | 4.4  |
| 30  | RG    | 135  | LEU  | 4.4  |
| 13  | XM    | 27   | LYS  | 4.4  |
| 5   | QE    | 125  | SER  | 4.4  |
| 28  | RE    | 60   | ASN  | 4.4  |
| 30  | YG    | 15   | VAL  | 4.4  |
| 51  | R5    | 2    | ALA  | 4.3  |
| 2   | QB    | 41   | ILE  | 4.3  |
| 25  | RA    | 1063 | G    | 4.3  |
| 30  | YG    | 103  | LEU  | 4.3  |
| 25  | RA    | 2119 | A    | 4.3  |
| 36  | YQ    | 21   | THR  | 4.3  |
| 25  | RA    | 1535 | U    | 4.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | R6    | 20   | ASN  | 4.3  |
| 4   | XD    | 2    | GLY  | 4.3  |
| 19  | XS    | 16   | LEU  | 4.3  |
| 35  | RP    | 14   | LYS  | 4.3  |
| 44  | YY    | 71   | LYS  | 4.3  |
| 12  | QL    | 16   | GLU  | 4.3  |
| 10  | XJ    | 45   | ARG  | 4.3  |
| 31  | YH    | 152  | ARG  | 4.3  |
| 21  | QU    | 14   | TRP  | 4.3  |
| 16  | XP    | 15   | PRO  | 4.3  |
| 35  | RP    | 87   | ASP  | 4.3  |
| 25  | YA    | 2119 | A    | 4.3  |
| 35  | RP    | 76   | LYS  | 4.3  |
| 30  | RG    | 176  | LEU  | 4.3  |
| 30  | RG    | 16   | ARG  | 4.3  |
| 28  | YE    | 56   | PRO  | 4.3  |
| 10  | XJ    | 64   | GLU  | 4.3  |
| 30  | RG    | 137  | GLU  | 4.3  |
| 23  | XY    | 32   | U    | 4.3  |
| 30  | RG    | 160  | VAL  | 4.3  |
| 41  | RV    | 45   | THR  | 4.3  |
| 7   | QG    | 4    | ARG  | 4.3  |
| 4   | QD    | 134  | ASP  | 4.3  |
| 36  | RQ    | 24   | GLY  | 4.3  |
| 30  | YG    | 41   | GLN  | 4.3  |
| 31  | YH    | 49   | VAL  | 4.3  |
| 51  | R5    | 57   | VAL  | 4.3  |
| 25  | RA    | 1069 | A    | 4.2  |
| 30  | YG    | 107  | LEU  | 4.2  |
| 30  | YG    | 65   | GLY  | 4.2  |
| 35  | RP    | 104  | GLY  | 4.2  |
| 14  | QN    | 46   | GLU  | 4.2  |
| 44  | RY    | 62   | GLU  | 4.2  |
| 52  | Y6    | 40   | CYS  | 4.2  |
| 50  | R4    | 9    | LEU  | 4.2  |
| 13  | XM    | 10   | PRO  | 4.2  |
| 10  | QJ    | 6    | ILE  | 4.2  |
| 1   | QA    | 1240 | U    | 4.2  |
| 10  | QJ    | 52   | GLY  | 4.2  |
| 25  | YA    | 2801 | A    | 4.2  |
| 34  | RO    | 55   | GLY  | 4.2  |
| 54  | R8    | 40   | GLU  | 4.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 28         | RE           | 69         | LYS         | 4.2         |
| 36         | RQ           | 25         | ASP         | 4.2         |
| 52         | R6           | 27         | LYS         | 4.2         |
| 5          | XE           | 123        | LEU         | 4.2         |
| 13         | XM           | 100        | GLY         | 4.2         |
| 54         | Y8           | 40         | GLU         | 4.2         |
| 30         | RG           | 37         | VAL         | 4.2         |
| 28         | YE           | 60         | ASN         | 4.2         |
| 54         | R8           | 61         | LEU         | 4.2         |
| 31         | YH           | 75         | ALA         | 4.2         |
| 32         | RI           | 8          | PRO         | 4.2         |
| 44         | RY           | 103        | GLY         | 4.2         |
| 10         | QJ           | 55         | LYS         | 4.2         |
| 50         | Y4           | 34         | GLU         | 4.2         |
| 30         | YG           | 153        | ARG         | 4.2         |
| 35         | YP           | 15         | ARG         | 4.2         |
| 30         | YG           | 111        | LEU         | 4.2         |
| 30         | YG           | 152        | LEU         | 4.2         |
| 30         | YG           | 132        | ASN         | 4.2         |
| 55         | R9           | 34         | GLN         | 4.2         |
| 30         | RG           | 158        | ALA         | 4.2         |
| 13         | XM           | 6          | GLY         | 4.2         |
| 20         | XT           | 79         | ARG         | 4.2         |
| 30         | RG           | 38         | VAL         | 4.1         |
| 50         | R4           | 68         | ARG         | 4.2         |
| 52         | R6           | 18         | ARG         | 4.2         |
| 30         | YG           | 137        | GLU         | 4.1         |
| 54         | R8           | 48         | PHE         | 4.1         |
| 30         | RG           | 57         | ALA         | 4.1         |
| 51         | Y5           | 2          | ALA         | 4.1         |
| 35         | RP           | 108        | LYS         | 4.1         |
| 41         | YV           | 41         | GLY         | 4.1         |
| 1          | QA           | 1451       | A           | 4.1         |
| 2          | QB           | 217        | ARG         | 4.1         |
| 8          | XH           | 3          | THR         | 4.1         |
| 14         | QN           | 41         | ARG         | 4.1         |
| 10         | XJ           | 98         | ILE         | 4.1         |
| 14         | XN           | 42         | ILE         | 4.1         |
| 30         | YG           | 130        | ASN         | 4.1         |
| 38         | RS           | 2          | ALA         | 4.1         |
| 52         | Y6           | 22         | ALA         | 4.1         |
| 31         | RH           | 63         | SER         | 4.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | XD    | 73   | ARG  | 4.1  |
| 36  | YQ    | 19   | GLY  | 4.1  |
| 53  | R7    | 1    | MET  | 4.1  |
| 53  | Y7    | 1    | MET  | 4.1  |
| 12  | QL    | 129  | ALA  | 4.1  |
| 2   | QB    | 97   | TRP  | 4.1  |
| 44  | YY    | 82   | PRO  | 4.1  |
| 43  | RX    | 60   | ARG  | 4.1  |
| 45  | YZ    | 87   | ASP  | 4.1  |
| 50  | Y4    | 51   | ASP  | 4.1  |
| 10  | QJ    | 72   | VAL  | 4.1  |
| 44  | YY    | 49   | VAL  | 4.1  |
| 3   | QC    | 15   | THR  | 4.1  |
| 31  | YH    | 47   | GLU  | 4.1  |
| 37  | YR    | 102  | GLU  | 4.1  |
| 15  | XO    | 2    | PRO  | 4.1  |
| 38  | RS    | 20   | ARG  | 4.1  |
| 53  | R7    | 41   | ARG  | 4.1  |
| 1   | QA    | 532  | A    | 4.1  |
| 56  | Z8    | 75   | C    | 4.1  |
| 34  | RO    | 122  | LEU  | 4.1  |
| 10  | XJ    | 55   | LYS  | 4.1  |
| 30  | RG    | 12   | TYR  | 4.1  |
| 47  | R1    | 96   | LYS  | 4.1  |
| 2   | QB    | 141  | GLU  | 4.1  |
| 3   | XC    | 161  | GLU  | 4.1  |
| 27  | YD    | 30   | GLU  | 4.1  |
| 44  | YY    | 2    | ARG  | 4.1  |
| 1   | XA    | 1125 | U    | 4.1  |
| 25  | YA    | 1535 | U    | 4.1  |
| 33  | RN    | 131  | GLN  | 4.1  |
| 16  | QP    | 15   | PRO  | 4.1  |
| 30  | RG    | 17   | PRO  | 4.1  |
| 14  | QN    | 25   | VAL  | 4.0  |
| 25  | RA    | 1103 | A    | 4.0  |
| 36  | RQ    | 129  | THR  | 4.0  |
| 34  | RO    | 47   | ILE  | 4.0  |
| 5   | QE    | 25   | ARG  | 4.0  |
| 30  | RG    | 91   | ARG  | 4.0  |
| 31  | YH    | 169  | VAL  | 4.0  |
| 40  | RU    | 90   | VAL  | 4.0  |
| 7   | XG    | 37   | ASN  | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | YD    | 122  | ASP  | 4.0  |
| 45  | RZ    | 149  | SER  | 4.0  |
| 45  | YZ    | 148  | ASP  | 4.0  |
| 11  | QK    | 25   | TYR  | 4.0  |
| 30  | YG    | 114  | ILE  | 4.0  |
| 14  | QN    | 3    | ARG  | 4.0  |
| 30  | YG    | 164  | GLU  | 4.0  |
| 25  | RA    | 1084 | A    | 4.0  |
| 30  | RG    | 82   | LEU  | 4.0  |
| 45  | RZ    | 78   | LYS  | 4.0  |
| 1   | XA    | 1126 | U    | 4.0  |
| 17  | QQ    | 81   | ARG  | 4.0  |
| 50  | R4    | 14   | ILE  | 4.0  |
| 4   | XD    | 24   | GLU  | 4.0  |
| 28  | RE    | 68   | ALA  | 4.0  |
| 11  | QK    | 127  | LYS  | 4.0  |
| 18  | QR    | 88   | LYS  | 4.0  |
| 48  | R2    | 9    | GLN  | 4.0  |
| 49  | R3    | 2    | PRO  | 4.0  |
| 25  | RA    | 1537 | C    | 4.0  |
| 20  | QT    | 75   | ASN  | 4.0  |
| 52  | R6    | 7    | ILE  | 4.0  |
| 17  | XQ    | 78   | GLU  | 4.0  |
| 39  | RT    | 46   | GLU  | 4.0  |
| 25  | YA    | 614  | U    | 4.0  |
| 2   | XB    | 238  | LEU  | 4.0  |
| 30  | RG    | 106  | LEU  | 4.0  |
| 50  | Y4    | 69   | LYS  | 4.0  |
| 12  | QL    | 18   | VAL  | 4.0  |
| 45  | RZ    | 180  | VAL  | 4.0  |
| 5   | QE    | 85   | GLY  | 4.0  |
| 28  | RE    | 66   | HIS  | 4.0  |
| 22  | XV    | 1    | C    | 4.0  |
| 51  | Y5    | 51   | TYR  | 4.0  |
| 19  | XS    | 42   | PRO  | 3.9  |
| 9   | XI    | 3    | GLN  | 3.9  |
| 27  | RD    | 236  | GLY  | 3.9  |
| 44  | RY    | 50   | ARG  | 3.9  |
| 28  | RE    | 205  | ALA  | 3.9  |
| 16  | XP    | 67   | THR  | 3.9  |
| 25  | YA    | 2126 | A    | 3.9  |
| 10  | QJ    | 37   | PRO  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | YA    | 2174 | C    | 3.9  |
| 30  | RG    | 89   | GLY  | 3.9  |
| 25  | YA    | 2118 | U    | 3.9  |
| 13  | XM    | 31   | LYS  | 3.9  |
| 30  | RG    | 61   | ALA  | 3.9  |
| 30  | YG    | 90   | LEU  | 3.9  |
| 30  | YG    | 139  | LEU  | 3.9  |
| 35  | YP    | 110  | TYR  | 3.9  |
| 13  | QM    | 32   | GLU  | 3.9  |
| 36  | YQ    | 91   | GLU  | 3.9  |
| 31  | YH    | 50   | VAL  | 3.9  |
| 2   | XB    | 160  | ASP  | 3.9  |
| 31  | YH    | 134  | SER  | 3.9  |
| 13  | XM    | 24   | GLY  | 3.9  |
| 21  | XU    | 2    | GLY  | 3.9  |
| 51  | R5    | 34   | PRO  | 3.9  |
| 25  | RA    | 2894 | G    | 3.9  |
| 51  | R5    | 49   | CYS  | 3.9  |
| 52  | Y6    | 16   | CYS  | 3.9  |
| 54  | Y8    | 34   | TRP  | 3.9  |
| 5   | QE    | 81   | GLU  | 3.9  |
| 10  | XJ    | 46   | ARG  | 3.9  |
| 30  | YG    | 95   | ARG  | 3.9  |
| 11  | XK    | 26   | ASN  | 3.9  |
| 36  | YQ    | 139  | GLU  | 3.9  |
| 2   | XB    | 195  | ASP  | 3.9  |
| 45  | RZ    | 140  | ASP  | 3.9  |
| 30  | RG    | 138  | GLN  | 3.9  |
| 31  | YH    | 4    | ILE  | 3.9  |
| 10  | QJ    | 62   | HIS  | 3.9  |
| 25  | RA    | 1089 | G    | 3.9  |
| 30  | YG    | 131  | TYR  | 3.9  |
| 56  | Z6    | 75   | C    | 3.9  |
| 4   | XD    | 150  | GLU  | 3.9  |
| 29  | RF    | 136  | THR  | 3.9  |
| 45  | RZ    | 168  | GLU  | 3.9  |
| 25  | RA    | 12   | U    | 3.9  |
| 30  | YG    | 68   | PRO  | 3.9  |
| 40  | RU    | 97   | ASP  | 3.9  |
| 30  | YG    | 60   | LEU  | 3.9  |
| 31  | RH    | 64   | LEU  | 3.9  |
| 44  | RY    | 16   | ALA  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | R9    | 22   | ARG  | 3.8  |
| 45  | RZ    | 175  | VAL  | 3.8  |
| 2   | QB    | 12   | GLU  | 3.8  |
| 52  | R6    | 39   | TYR  | 3.8  |
| 15  | QO    | 2    | PRO  | 3.8  |
| 30  | YG    | 80   | PHE  | 3.8  |
| 21  | QU    | 5    | ASP  | 3.8  |
| 30  | RG    | 126  | ASP  | 3.8  |
| 2   | QB    | 187  | LEU  | 3.8  |
| 30  | RG    | 3    | LEU  | 3.8  |
| 14  | XN    | 25   | VAL  | 3.8  |
| 51  | R5    | 51   | TYR  | 3.8  |
| 7   | XG    | 82   | GLY  | 3.8  |
| 30  | YG    | 82   | LEU  | 3.8  |
| 20  | QT    | 8    | ARG  | 3.8  |
| 25  | RA    | 2118 | U    | 3.8  |
| 25  | RA    | 1087 | G    | 3.8  |
| 43  | RX    | 53   | LYS  | 3.8  |
| 44  | RY    | 47   | LYS  | 3.8  |
| 47  | R1    | 92   | LYS  | 3.8  |
| 55  | R9    | 15   | LYS  | 3.8  |
| 50  | R4    | 25   | TYR  | 3.8  |
| 2   | QB    | 39   | ILE  | 3.8  |
| 10  | QJ    | 74   | ILE  | 3.8  |
| 52  | R6    | 41   | PRO  | 3.8  |
| 19  | XS    | 30   | LEU  | 3.8  |
| 52  | Y6    | 18   | ARG  | 3.8  |
| 10  | QJ    | 20   | ALA  | 3.8  |
| 13  | QM    | 2    | ALA  | 3.8  |
| 30  | RG    | 73   | ALA  | 3.8  |
| 44  | RY    | 3    | VAL  | 3.8  |
| 9   | QI    | 95   | LYS  | 3.8  |
| 50  | R4    | 28   | LYS  | 3.8  |
| 51  | R5    | 3    | LYS  | 3.8  |
| 25  | RA    | 529  | A    | 3.8  |
| 25  | RA    | 1510 | A    | 3.8  |
| 1   | QA    | 1159 | U    | 3.8  |
| 10  | XJ    | 6    | ILE  | 3.8  |
| 25  | RA    | 2798 | C    | 3.8  |
| 29  | RF    | 207  | GLY  | 3.8  |
| 30  | YG    | 39   | ILE  | 3.8  |
| 10  | XJ    | 43   | ARG  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | YE    | 76   | ARG  | 3.8  |
| 1   | XA    | 438  | G    | 3.8  |
| 25  | YA    | 1110 | G    | 3.8  |
| 2   | XB    | 16   | HIS  | 3.8  |
| 40  | YU    | 85   | LYS  | 3.8  |
| 16  | XP    | 29   | ASP  | 3.8  |
| 38  | YS    | 88   | ASP  | 3.8  |
| 29  | YF    | 131  | GLY  | 3.8  |
| 4   | XD    | 97   | LEU  | 3.8  |
| 25  | RA    | 2799 | A    | 3.8  |
| 4   | QD    | 12   | CYS  | 3.8  |
| 5   | XE    | 62   | ALA  | 3.7  |
| 25  | RA    | 34   | C    | 3.7  |
| 2   | QB    | 136  | VAL  | 3.7  |
| 21  | XU    | 5    | ASP  | 3.7  |
| 25  | RA    | 1071 | G    | 3.7  |
| 30  | YG    | 52   | ILE  | 3.7  |
| 3   | QC    | 91   | LEU  | 3.7  |
| 8   | XH    | 90   | GLY  | 3.7  |
| 39  | YT    | 21   | GLU  | 3.7  |
| 51  | Y5    | 59   | GLU  | 3.7  |
| 28  | YE    | 205  | ALA  | 3.7  |
| 30  | YG    | 171  | ALA  | 3.7  |
| 38  | YS    | 2    | ALA  | 3.7  |
| 2   | XB    | 15   | VAL  | 3.7  |
| 17  | QQ    | 93   | GLN  | 3.7  |
| 1   | QA    | 1130 | A    | 3.7  |
| 55  | Y9    | 20   | HIS  | 3.7  |
| 22  | QV    | 1    | C    | 3.7  |
| 14  | QN    | 12   | ARG  | 3.7  |
| 10  | QJ    | 64   | GLU  | 3.7  |
| 15  | QO    | 26   | GLU  | 3.7  |
| 39  | RT    | 24   | PRO  | 3.7  |
| 3   | QC    | 149  | ALA  | 3.7  |
| 13  | QM    | 15   | VAL  | 3.7  |
| 30  | YG    | 28   | VAL  | 3.7  |
| 4   | XD    | 12   | CYS  | 3.7  |
| 21  | QU    | 24   | ARG  | 3.7  |
| 25  | RA    | 614  | U    | 3.7  |
| 12  | XL    | 16   | GLU  | 3.7  |
| 35  | RP    | 117  | GLU  | 3.7  |
| 12  | XL    | 129  | ALA  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | YG    | 57   | ALA  | 3.7  |
| 30  | YG    | 5    | VAL  | 3.7  |
| 5   | QE    | 24   | ARG  | 3.7  |
| 2   | QB    | 140  | HIS  | 3.7  |
| 44  | YY    | 99   | CYS  | 3.7  |
| 3   | XC    | 196  | LEU  | 3.7  |
| 21  | XU    | 16   | GLY  | 3.7  |
| 30  | YG    | 134  | GLY  | 3.7  |
| 50  | R4    | 42   | PHE  | 3.7  |
| 50  | R4    | 70   | GLY  | 3.7  |
| 19  | XS    | 76   | PRO  | 3.7  |
| 25  | YA    | 1026 | U    | 3.7  |
| 45  | RZ    | 176  | PRO  | 3.7  |
| 4   | QD    | 15   | GLU  | 3.7  |
| 9   | QI    | 105  | ASP  | 3.7  |
| 53  | R7    | 45   | ALA  | 3.7  |
| 41  | YV    | 14   | VAL  | 3.7  |
| 53  | R7    | 47   | ARG  | 3.7  |
| 30  | RG    | 107  | LEU  | 3.7  |
| 45  | YZ    | 155  | LEU  | 3.7  |
| 20  | XT    | 9    | ASN  | 3.7  |
| 13  | QM    | 113  | PRO  | 3.6  |
| 30  | YG    | 87   | PRO  | 3.6  |
| 10  | QJ    | 49   | VAL  | 3.6  |
| 25  | YA    | 2116 | G    | 3.6  |
| 32  | RI    | 110  | ASP  | 3.6  |
| 50  | Y4    | 63   | TYR  | 3.6  |
| 13  | XM    | 102  | ARG  | 3.6  |
| 5   | XE    | 98   | THR  | 3.6  |
| 54  | R8    | 27   | THR  | 3.6  |
| 4   | QD    | 158  | ILE  | 3.6  |
| 36  | YQ    | 79   | LEU  | 3.6  |
| 13  | QM    | 121  | LYS  | 3.6  |
| 18  | XR    | 88   | LYS  | 3.6  |
| 1   | QA    | 466  | C    | 3.6  |
| 9   | XI    | 111  | ARG  | 3.6  |
| 29  | RF    | 56   | GLU  | 3.6  |
| 30  | RG    | 11   | TYR  | 3.6  |
| 30  | RG    | 98   | ARG  | 3.6  |
| 30  | RG    | 151  | ALA  | 3.6  |
| 50  | Y4    | 33   | VAL  | 3.6  |
| 41  | YV    | 26   | ASP  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | RG    | 120  | LEU  | 3.6  |
| 7   | QG    | 86   | GLN  | 3.6  |
| 36  | RQ    | 87   | LYS  | 3.6  |
| 1   | XA    | 630  | G    | 3.6  |
| 30  | YG    | 125  | PHE  | 3.6  |
| 50  | Y4    | 49   | PHE  | 3.6  |
| 30  | YG    | 154  | GLY  | 3.6  |
| 47  | R1    | 79   | GLY  | 3.6  |
| 25  | YA    | 887  | A    | 3.6  |
| 10  | XJ    | 37   | PRO  | 3.6  |
| 20  | XT    | 75   | ASN  | 3.6  |
| 30  | RG    | 123  | ASN  | 3.6  |
| 52  | Y6    | 13   | CYS  | 3.6  |
| 35  | YP    | 16   | ARG  | 3.6  |
| 49  | R3    | 30   | ARG  | 3.6  |
| 25  | YA    | 2896 | C    | 3.6  |
| 30  | YG    | 70   | VAL  | 3.6  |
| 30  | YG    | 99   | MET  | 3.6  |
| 45  | YZ    | 166  | SER  | 3.6  |
| 9   | XI    | 11   | LYS  | 3.6  |
| 10  | QJ    | 88   | LEU  | 3.6  |
| 17  | XQ    | 83   | ASP  | 3.6  |
| 31  | RH    | 171  | LEU  | 3.6  |
| 31  | YH    | 100  | GLY  | 3.6  |
| 42  | RW    | 112  | GLY  | 3.6  |
| 35  | RP    | 15   | ARG  | 3.6  |
| 10  | QJ    | 34   | VAL  | 3.6  |
| 14  | QN    | 24   | CYS  | 3.6  |
| 25  | RA    | 2125 | G    | 3.6  |
| 47  | R1    | 97   | LEU  | 3.6  |
| 50  | R4    | 2    | LYS  | 3.6  |
| 40  | RU    | 91   | ASP  | 3.6  |
| 44  | YY    | 89   | PHE  | 3.6  |
| 7   | QG    | 5    | ARG  | 3.6  |
| 7   | XG    | 4    | ARG  | 3.6  |
| 11  | XK    | 49   | GLY  | 3.6  |
| 13  | QM    | 102  | ARG  | 3.6  |
| 37  | RR    | 46   | GLY  | 3.6  |
| 10  | XJ    | 24   | VAL  | 3.6  |
| 51  | R5    | 53   | ALA  | 3.6  |
| 7   | XG    | 8    | GLU  | 3.6  |
| 30  | RG    | 74   | LYS  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | YY    | 88   | LYS  | 3.6  |
| 30  | RG    | 140  | ILE  | 3.6  |
| 45  | RZ    | 137  | ILE  | 3.6  |
| 36  | RQ    | 135  | ASP  | 3.6  |
| 2   | QB    | 144  | ARG  | 3.5  |
| 9   | QI    | 66   | ARG  | 3.5  |
| 15  | QO    | 88   | ARG  | 3.5  |
| 25  | RA    | 276  | A    | 3.5  |
| 25  | YA    | 2892 | A    | 3.5  |
| 1   | QA    | 1054 | C    | 3.5  |
| 25  | YA    | 1537 | C    | 3.5  |
| 16  | QP    | 51   | VAL  | 3.5  |
| 28  | RE    | 7    | VAL  | 3.5  |
| 4   | XD    | 156  | GLU  | 3.5  |
| 39  | YT    | 109  | GLU  | 3.5  |
| 12  | XL    | 64   | TYR  | 3.5  |
| 48  | Y2    | 71   | ASN  | 3.5  |
| 4   | QD    | 73   | ARG  | 3.5  |
| 27  | YD    | 13   | ARG  | 3.5  |
| 35  | RP    | 61   | ARG  | 3.5  |
| 37  | YR    | 91   | GLN  | 3.5  |
| 6   | QF    | 40   | VAL  | 3.5  |
| 27  | YD    | 35   | LYS  | 3.5  |
| 30  | RG    | 31   | VAL  | 3.5  |
| 43  | RX    | 63   | LYS  | 3.5  |
| 44  | RY    | 87   | LYS  | 3.5  |
| 1   | XA    | 1451 | A    | 3.5  |
| 16  | QP    | 48   | TRP  | 3.5  |
| 45  | RZ    | 51   | ALA  | 3.5  |
| 39  | YT    | 1    | MET  | 3.5  |
| 47  | R1    | 94   | LEU  | 3.5  |
| 50  | Y4    | 9    | LEU  | 3.5  |
| 52  | Y6    | 11   | LEU  | 3.5  |
| 2   | XB    | 200  | ILE  | 3.5  |
| 3   | QC    | 35   | GLU  | 3.5  |
| 5   | QE    | 80   | ILE  | 3.5  |
| 30  | YG    | 14   | GLU  | 3.5  |
| 32  | YI    | 7    | GLU  | 3.5  |
| 52  | R6    | 12   | GLU  | 3.5  |
| 11  | QK    | 50   | TYR  | 3.5  |
| 30  | RG    | 27   | ASN  | 3.5  |
| 4   | XD    | 115  | ARG  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | XE    | 18   | ARG  | 3.5  |
| 4   | XD    | 31   | CYS  | 3.5  |
| 44  | RY    | 79   | CYS  | 3.5  |
| 11  | QK    | 87   | THR  | 3.5  |
| 12  | QL    | 32   | PHE  | 3.5  |
| 25  | RA    | 1065 | U    | 3.5  |
| 55  | R9    | 6    | SER  | 3.5  |
| 11  | XK    | 36   | ASP  | 3.5  |
| 27  | YD    | 71   | ASP  | 3.5  |
| 37  | RR    | 7    | GLY  | 3.5  |
| 47  | Y1    | 36   | GLY  | 3.5  |
| 50  | R4    | 12   | ALA  | 3.5  |
| 9   | XI    | 81   | ILE  | 3.5  |
| 28  | YE    | 77   | ILE  | 3.5  |
| 34  | RO    | 69   | ILE  | 3.5  |
| 16  | QP    | 18   | ARG  | 3.5  |
| 30  | YG    | 168  | GLU  | 3.5  |
| 1   | QA    | 1183 | A    | 3.5  |
| 39  | YT    | 2    | ASN  | 3.5  |
| 14  | QN    | 15   | LYS  | 3.5  |
| 44  | RY    | 94   | LYS  | 3.5  |
| 51  | Y5    | 49   | CYS  | 3.5  |
| 3   | QC    | 194  | GLY  | 3.5  |
| 44  | RY    | 51   | VAL  | 3.5  |
| 52  | Y6    | 5    | VAL  | 3.5  |
| 30  | RG    | 116  | ASP  | 3.5  |
| 30  | RG    | 2    | PRO  | 3.5  |
| 45  | RZ    | 117  | LEU  | 3.5  |
| 47  | Y1    | 97   | LEU  | 3.5  |
| 44  | RY    | 86   | ARG  | 3.5  |
| 41  | YV    | 53   | GLU  | 3.5  |
| 11  | QK    | 123  | LYS  | 3.5  |
| 14  | QN    | 36   | PHE  | 3.5  |
| 50  | Y4    | 2    | LYS  | 3.5  |
| 13  | QM    | 85   | GLY  | 3.5  |
| 14  | QN    | 38   | GLY  | 3.5  |
| 17  | XQ    | 93   | GLN  | 3.5  |
| 25  | YA    | 1084 | A    | 3.5  |
| 8   | QH    | 112  | LEU  | 3.5  |
| 44  | RY    | 52   | SER  | 3.5  |
| 47  | R1    | 77   | ALA  | 3.5  |
| 1   | QA    | 1001 | G    | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | QO    | 68   | ARG  | 3.5  |
| 30  | YG    | 136  | ARG  | 3.5  |
| 45  | RZ    | 72   | ARG  | 3.5  |
| 52  | Y6    | 7    | ILE  | 3.5  |
| 25  | RA    | 2802 | G    | 3.5  |
| 2   | XB    | 12   | GLU  | 3.4  |
| 10  | QJ    | 7    | LYS  | 3.4  |
| 52  | Y6    | 8    | LYS  | 3.4  |
| 31  | YH    | 82   | GLY  | 3.4  |
| 31  | YH    | 122  | THR  | 3.4  |
| 38  | RS    | 60   | GLY  | 3.4  |
| 44  | RY    | 57   | GLN  | 3.4  |
| 7   | QG    | 79   | ARG  | 3.4  |
| 9   | QI    | 104  | ARG  | 3.4  |
| 29  | YF    | 205  | ARG  | 3.4  |
| 31  | RH    | 3    | ARG  | 3.4  |
| 31  | YH    | 8    | PRO  | 3.4  |
| 45  | RZ    | 159  | PRO  | 3.4  |
| 45  | YZ    | 130  | PRO  | 3.4  |
| 25  | RA    | 890  | A    | 3.4  |
| 20  | QT    | 74   | LYS  | 3.4  |
| 5   | QE    | 83   | GLU  | 3.4  |
| 5   | XE    | 81   | GLU  | 3.4  |
| 9   | XI    | 12   | GLU  | 3.4  |
| 25  | YA    | 2803 | C    | 3.4  |
| 30  | RG    | 105  | LYS  | 3.4  |
| 31  | RH    | 123  | PHE  | 3.4  |
| 54  | Y8    | 48   | PHE  | 3.4  |
| 9   | XI    | 114  | TYR  | 3.4  |
| 50  | Y4    | 32   | TYR  | 3.4  |
| 1   | QA    | 388  | G    | 3.4  |
| 1   | XA    | 64   | G    | 3.4  |
| 1   | XA    | 81   | G    | 3.4  |
| 5   | QE    | 67   | VAL  | 3.4  |
| 49  | R3    | 4    | LEU  | 3.4  |
| 52  | Y6    | 9    | LEU  | 3.4  |
| 50  | R4    | 27   | THR  | 3.4  |
| 3   | QC    | 6    | HIS  | 3.4  |
| 10  | XJ    | 33   | GLN  | 3.4  |
| 13  | XM    | 94   | ARG  | 3.4  |
| 17  | XQ    | 15   | MET  | 3.4  |
| 27  | YD    | 262  | ARG  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | RP    | 90   | ARG  | 3.4  |
| 14  | XN    | 43   | CYS  | 3.4  |
| 31  | RH    | 155  | SER  | 3.4  |
| 52  | R6    | 45   | LYS  | 3.4  |
| 14  | XN    | 46   | GLU  | 3.4  |
| 1   | QA    | 1032 | A    | 3.4  |
| 1   | QA    | 1286 | A    | 3.4  |
| 25  | RA    | 2173 | A    | 3.4  |
| 30  | RG    | 146  | TYR  | 3.4  |
| 30  | YG    | 11   | TYR  | 3.4  |
| 31  | RH    | 125  | VAL  | 3.4  |
| 30  | YG    | 120  | LEU  | 3.4  |
| 11  | QK    | 54   | ARG  | 3.4  |
| 16  | XP    | 71   | ARG  | 3.4  |
| 20  | XT    | 106  | ALA  | 3.4  |
| 27  | YD    | 176  | ARG  | 3.4  |
| 45  | RZ    | 113  | ALA  | 3.4  |
| 2   | XB    | 5    | ILE  | 3.4  |
| 13  | XM    | 101  | GLN  | 3.4  |
| 39  | RT    | 2    | ASN  | 3.4  |
| 52  | Y6    | 41   | PRO  | 3.4  |
| 51  | R5    | 40   | LYS  | 3.4  |
| 25  | RA    | 2121 | G    | 3.4  |
| 25  | YA    | 1056 | G    | 3.4  |
| 7   | XG    | 77   | SER  | 3.4  |
| 30  | YG    | 29   | TRP  | 3.4  |
| 13  | QM    | 8    | GLU  | 3.4  |
| 17  | QQ    | 24   | GLU  | 3.4  |
| 30  | YG    | 180  | PHE  | 3.4  |
| 39  | YT    | 11   | GLU  | 3.4  |
| 50  | R4    | 34   | GLU  | 3.4  |
| 30  | RG    | 152  | LEU  | 3.4  |
| 17  | QQ    | 91   | ARG  | 3.4  |
| 31  | YH    | 6    | ARG  | 3.4  |
| 1   | XA    | 197  | A    | 3.4  |
| 25  | RA    | 2629 | A    | 3.4  |
| 30  | RG    | 20   | ILE  | 3.4  |
| 50  | Y4    | 31   | ILE  | 3.4  |
| 2   | XB    | 110  | GLN  | 3.4  |
| 28  | RE    | 54   | GLN  | 3.4  |
| 37  | RR    | 91   | GLN  | 3.4  |
| 45  | RZ    | 55   | HIS  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | QD    | 29   | PRO  | 3.4  |
| 36  | RQ    | 99   | PRO  | 3.4  |
| 52  | Y6    | 27   | LYS  | 3.4  |
| 25  | RA    | 1078 | U    | 3.4  |
| 10  | XJ    | 54   | PHE  | 3.4  |
| 9   | XI    | 10   | ARG  | 3.4  |
| 10  | XJ    | 72   | VAL  | 3.4  |
| 31  | YH    | 46   | GLU  | 3.4  |
| 32  | YI    | 15   | VAL  | 3.4  |
| 36  | RQ    | 138  | ASP  | 3.4  |
| 36  | RQ    | 139  | GLU  | 3.4  |
| 45  | RZ    | 169  | GLU  | 3.4  |
| 12  | QL    | 41   | ARG  | 3.4  |
| 52  | R6    | 50   | ARG  | 3.4  |
| 1   | QA    | 81   | G    | 3.4  |
| 25  | RA    | 1044 | G    | 3.4  |
| 9   | XI    | 72   | GLY  | 3.4  |
| 14  | QN    | 30   | ALA  | 3.4  |
| 45  | RZ    | 114  | GLY  | 3.4  |
| 30  | YG    | 144  | ILE  | 3.4  |
| 25  | YA    | 1103 | A    | 3.3  |
| 16  | XP    | 48   | TRP  | 3.3  |
| 10  | XJ    | 85   | LEU  | 3.3  |
| 17  | QQ    | 35   | VAL  | 3.3  |
| 25  | RA    | 279  | C    | 3.3  |
| 30  | RG    | 149  | VAL  | 3.3  |
| 55  | Y9    | 3    | VAL  | 3.3  |
| 55  | Y9    | 9    | ARG  | 3.3  |
| 19  | QS    | 13   | ASP  | 3.3  |
| 30  | YG    | 156  | ASP  | 3.3  |
| 36  | YQ    | 138  | ASP  | 3.3  |
| 9   | QI    | 36   | TYR  | 3.3  |
| 2   | QB    | 80   | ILE  | 3.3  |
| 28  | RE    | 77   | ILE  | 3.3  |
| 13  | QM    | 97   | PRO  | 3.3  |
| 19  | QS    | 69   | HIS  | 3.3  |
| 1   | QA    | 1003 | G    | 3.3  |
| 1   | QA    | 1033 | G    | 3.3  |
| 1   | XA    | 1124 | G    | 3.3  |
| 24  | QX    | 6    | G    | 3.3  |
| 25  | YA    | 1176 | G    | 3.3  |
| 4   | QD    | 209  | ARG  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | QG    | 141  | VAL  | 3.3  |
| 28  | YE    | 21   | VAL  | 3.3  |
| 33  | YN    | 138  | LEU  | 3.3  |
| 45  | RZ    | 105  | VAL  | 3.3  |
| 47  | R1    | 70   | VAL  | 3.3  |
| 51  | R5    | 59   | GLU  | 3.3  |
| 1   | XA    | 87   | A    | 3.3  |
| 4   | QD    | 22   | LYS  | 3.3  |
| 4   | XD    | 91   | SER  | 3.3  |
| 25  | YA    | 2135 | A    | 3.3  |
| 25  | YA    | 2170 | A    | 3.3  |
| 40  | YU    | 77   | SER  | 3.3  |
| 44  | RY    | 33   | LYS  | 3.3  |
| 30  | RG    | 25   | TYR  | 3.3  |
| 31  | YH    | 41   | MET  | 3.3  |
| 44  | RY    | 76   | CYS  | 3.3  |
| 10  | XJ    | 73   | ASP  | 3.3  |
| 25  | RA    | 1094 | U    | 3.3  |
| 30  | YG    | 112  | PRO  | 3.3  |
| 35  | RP    | 68   | GLN  | 3.3  |
| 52  | R6    | 26   | ASN  | 3.3  |
| 4   | XD    | 151  | LYS  | 3.3  |
| 20  | QT    | 34   | LYS  | 3.3  |
| 18  | QR    | 46   | GLU  | 3.3  |
| 1   | XA    | 181  | G    | 3.3  |
| 8   | QH    | 113  | SER  | 3.3  |
| 12  | QL    | 26   | ALA  | 3.3  |
| 27  | YD    | 236  | GLY  | 3.3  |
| 35  | YP    | 11   | GLY  | 3.3  |
| 41  | YV    | 4    | ILE  | 3.3  |
| 47  | R1    | 36   | GLY  | 3.3  |
| 3   | XC    | 193  | TYR  | 3.3  |
| 8   | QH    | 57   | PRO  | 3.3  |
| 25  | RA    | 860  | U    | 3.3  |
| 25  | RA    | 1082 | U    | 3.3  |
| 29  | RF    | 175  | THR  | 3.3  |
| 50  | Y4    | 6    | HIS  | 3.3  |
| 54  | R8    | 31   | HIS  | 3.3  |
| 55  | R9    | 35   | ARG  | 3.3  |
| 55  | Y9    | 32   | HIS  | 3.3  |
| 30  | RG    | 173  | LEU  | 3.3  |
| 31  | YH    | 76   | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | YI    | 118  | LYS  | 3.3  |
| 40  | YU    | 90   | VAL  | 3.3  |
| 41  | RV    | 14   | VAL  | 3.3  |
| 36  | RQ    | 1    | MET  | 3.3  |
| 13  | QM    | 84   | ILE  | 3.3  |
| 38  | RS    | 64   | GLU  | 3.3  |
| 41  | YV    | 23   | GLU  | 3.3  |
| 19  | QS    | 4    | SER  | 3.3  |
| 37  | RR    | 6    | SER  | 3.3  |
| 12  | QL    | 94   | PRO  | 3.3  |
| 14  | QN    | 31   | ARG  | 3.3  |
| 30  | RG    | 136  | ARG  | 3.3  |
| 39  | YT    | 115  | ARG  | 3.3  |
| 54  | R8    | 46   | ARG  | 3.3  |
| 1   | XA    | 1001 | G    | 3.3  |
| 12  | QL    | 46   | LYS  | 3.3  |
| 36  | RQ    | 63   | LYS  | 3.3  |
| 36  | RQ    | 81   | VAL  | 3.3  |
| 44  | YY    | 63   | LYS  | 3.3  |
| 25  | RA    | 1054 | A    | 3.3  |
| 4   | QD    | 200  | GLU  | 3.3  |
| 45  | RZ    | 146  | ILE  | 3.3  |
| 48  | Y2    | 11   | GLU  | 3.3  |
| 34  | RO    | 78   | ARG  | 3.2  |
| 40  | RU    | 59   | ARG  | 3.2  |
| 44  | RY    | 2    | ARG  | 3.2  |
| 9   | XI    | 126  | SER  | 3.2  |
| 16  | QP    | 16   | HIS  | 3.2  |
| 35  | YP    | 36   | LYS  | 3.2  |
| 36  | YQ    | 81   | VAL  | 3.2  |
| 20  | QT    | 12   | ALA  | 3.2  |
| 30  | RG    | 79   | ASN  | 3.2  |
| 42  | RW    | 5    | ALA  | 3.2  |
| 23  | QY    | 31   | G    | 3.2  |
| 25  | RA    | 1068 | G    | 3.2  |
| 25  | YA    | 12   | U    | 3.2  |
| 25  | YA    | 1058 | G    | 3.2  |
| 25  | YA    | 2120 | G    | 3.2  |
| 25  | YA    | 2805 | G    | 3.2  |
| 29  | YF    | 152  | GLU  | 3.2  |
| 50  | Y4    | 25   | TYR  | 3.2  |
| 1   | QA    | 980  | C    | 3.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 11         | QK           | 11         | LYS         | 3.2         |
| 19         | QS           | 32         | LYS         | 3.2         |
| 44         | RY           | 56         | PRO         | 3.2         |
| 51         | Y5           | 34         | PRO         | 3.2         |
| 2          | QB           | 105        | PHE         | 3.2         |
| 20         | QT           | 73         | HIS         | 3.2         |
| 37         | RR           | 47         | PHE         | 3.2         |
| 42         | YW           | 94         | ASP         | 3.2         |
| 14         | XN           | 22         | THR         | 3.2         |
| 31         | RH           | 122        | THR         | 3.2         |
| 7          | XG           | 83         | ALA         | 3.2         |
| 38         | RS           | 55         | ALA         | 3.2         |
| 40         | YU           | 116        | ALA         | 3.2         |
| 31         | YH           | 124        | GLU         | 3.2         |
| 36         | RQ           | 48         | GLU         | 3.2         |
| 36         | RQ           | 105        | GLU         | 3.2         |
| 39         | RT           | 37         | GLY         | 3.2         |
| 12         | QL           | 69         | TYR         | 3.2         |
| 15         | QO           | 48         | LYS         | 3.2         |
| 20         | QT           | 27         | LYS         | 3.2         |
| 30         | YG           | 146        | TYR         | 3.2         |
| 31         | YH           | 171        | LEU         | 3.2         |
| 45         | YZ           | 163        | LEU         | 3.2         |
| 51         | Y5           | 58         | LEU         | 3.2         |
| 52         | R6           | 9          | LEU         | 3.2         |
| 52         | Y6           | 38         | LYS         | 3.2         |
| 25         | RA           | 1026       | U           | 3.2         |
| 41         | RV           | 36         | PRO         | 3.2         |
| 1          | QA           | 1032(B)    | G           | 3.2         |
| 1          | QA           | 1181       | G           | 3.2         |
| 5          | QE           | 90         | VAL         | 3.2         |
| 9          | QI           | 18         | PHE         | 3.2         |
| 25         | RA           | 1073       | A           | 3.2         |
| 25         | YA           | 1059       | G           | 3.2         |
| 8          | XH           | 4          | ASP         | 3.2         |
| 30         | YG           | 161        | THR         | 3.2         |
| 30         | RG           | 144        | ILE         | 3.2         |
| 4          | XD           | 122        | ARG         | 3.2         |
| 30         | RG           | 113        | ARG         | 3.2         |
| 31         | YH           | 59         | ARG         | 3.2         |
| 32         | YI           | 50         | ARG         | 3.2         |
| 29         | RF           | 131        | GLY         | 3.2         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17  | QQ    | 78  | GLU  | 3.2  |
| 27  | RD    | 237 | GLU  | 3.2  |
| 12  | XL    | 17  | LYS  | 3.2  |
| 7   | QG    | 26  | PHE  | 3.2  |
| 27  | YD    | 15  | PHE  | 3.2  |
| 30  | RG    | 180 | PHE  | 3.2  |
| 44  | RY    | 77  | PRO  | 3.2  |
| 10  | XJ    | 34  | VAL  | 3.2  |
| 43  | RX    | 52  | VAL  | 3.2  |
| 52  | Y6    | 48  | VAL  | 3.2  |
| 55  | Y9    | 16  | VAL  | 3.2  |
| 25  | RA    | 161 | U    | 3.2  |
| 2   | XB    | 214 | ILE  | 3.2  |
| 12  | QL    | 44  | THR  | 3.2  |
| 45  | RZ    | 98  | MET  | 3.2  |
| 14  | QN    | 26  | ARG  | 3.2  |
| 14  | XN    | 3   | ARG  | 3.2  |
| 35  | YP    | 79  | ARG  | 3.2  |
| 14  | QN    | 27  | CYS  | 3.2  |
| 34  | RO    | 30  | ALA  | 3.2  |
| 55  | Y9    | 14  | CYS  | 3.2  |
| 35  | YP    | 121 | LYS  | 3.2  |
| 48  | Y2    | 15  | LYS  | 3.2  |
| 53  | Y7    | 32  | LYS  | 3.2  |
| 8   | XH    | 2   | LEU  | 3.2  |
| 17  | XQ    | 24  | GLU  | 3.2  |
| 28  | YE    | 163 | GLU  | 3.2  |
| 30  | YG    | 94  | LEU  | 3.2  |
| 34  | RO    | 29  | ASN  | 3.2  |
| 5   | QE    | 133 | TYR  | 3.2  |
| 30  | RG    | 178 | PHE  | 3.2  |
| 45  | YZ    | 167 | PRO  | 3.2  |
| 30  | YG    | 83  | ARG  | 3.2  |
| 30  | RG    | 124 | SER  | 3.2  |
| 2   | QB    | 188 | ALA  | 3.2  |
| 20  | XT    | 66  | ALA  | 3.2  |
| 39  | RT    | 97  | ALA  | 3.2  |
| 33  | YN    | 118 | LYS  | 3.1  |
| 35  | YP    | 108 | LYS  | 3.1  |
| 47  | R1    | 28  | GLY  | 3.1  |
| 51  | Y5    | 36  | CYS  | 3.1  |
| 10  | XJ    | 71  | LEU  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | QD    | 24   | GLU  | 3.1  |
| 4   | XD    | 80   | GLU  | 3.1  |
| 32  | YI    | 122  | GLU  | 3.1  |
| 37  | RR    | 43   | GLU  | 3.1  |
| 39  | RT    | 11   | GLU  | 3.1  |
| 25  | RA    | 1096 | A    | 3.1  |
| 25  | RA    | 2171 | A    | 3.1  |
| 11  | QK    | 26   | ASN  | 3.1  |
| 31  | YH    | 44   | VAL  | 3.1  |
| 40  | RU    | 2    | PRO  | 3.1  |
| 1   | XA    | 934  | C    | 3.1  |
| 23  | XY    | 31   | G    | 3.1  |
| 25  | RA    | 1110 | G    | 3.1  |
| 25  | YA    | 2112 | G    | 3.1  |
| 8   | QH    | 9    | MET  | 3.1  |
| 51  | Y5    | 40   | LYS  | 3.1  |
| 55  | Y9    | 31   | LYS  | 3.1  |
| 16  | QP    | 22   | THR  | 3.1  |
| 43  | RX    | 3    | THR  | 3.1  |
| 3   | XC    | 148  | GLY  | 3.1  |
| 17  | QQ    | 13   | ASP  | 3.1  |
| 19  | XS    | 5    | LEU  | 3.1  |
| 35  | RP    | 62   | LEU  | 3.1  |
| 38  | YS    | 41   | ASP  | 3.1  |
| 39  | YT    | 6    | LEU  | 3.1  |
| 51  | R5    | 46   | CYS  | 3.1  |
| 25  | RA    | 362  | U    | 3.1  |
| 10  | QJ    | 47   | PHE  | 3.1  |
| 30  | YG    | 37   | VAL  | 3.1  |
| 2   | QB    | 31   | TYR  | 3.1  |
| 47  | R1    | 21   | ARG  | 3.1  |
| 1   | XA    | 315  | A    | 3.1  |
| 20  | XT    | 21   | LYS  | 3.1  |
| 33  | YN    | 109  | LYS  | 3.1  |
| 29  | YF    | 58   | ALA  | 3.1  |
| 34  | RO    | 103  | ALA  | 3.1  |
| 12  | QL    | 88   | GLY  | 3.1  |
| 20  | XT    | 11   | SER  | 3.1  |
| 30  | YG    | 42   | GLY  | 3.1  |
| 16  | QP    | 29   | ASP  | 3.1  |
| 19  | XS    | 17   | GLU  | 3.1  |
| 47  | R1    | 27   | GLU  | 3.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | QB    | 164    | VAL  | 3.1  |
| 13  | XM    | 53     | VAL  | 3.1  |
| 19  | QS    | 41     | VAL  | 3.1  |
| 44  | YY    | 76     | CYS  | 3.1  |
| 4   | QD    | 132    | ARG  | 3.1  |
| 7   | QG    | 78     | ARG  | 3.1  |
| 12  | XL    | 5      | PRO  | 3.1  |
| 30  | YG    | 12     | TYR  | 3.1  |
| 4   | QD    | 151    | LYS  | 3.1  |
| 12  | XL    | 23     | LYS  | 3.1  |
| 25  | RA    | 271(C) | U    | 3.1  |
| 26  | RB    | 55     | U    | 3.1  |
| 54  | Y8    | 33     | ASN  | 3.1  |
| 9   | QI    | 3      | GLN  | 3.1  |
| 31  | YH    | 7      | LEU  | 3.1  |
| 52  | Y6    | 34     | LEU  | 3.1  |
| 16  | QP    | 69     | THR  | 3.1  |
| 25  | RA    | 2169   | A    | 3.1  |
| 29  | YF    | 48     | THR  | 3.1  |
| 30  | YG    | 124    | SER  | 3.1  |
| 3   | QC    | 161    | GLU  | 3.1  |
| 10  | QJ    | 58     | ASP  | 3.1  |
| 25  | RA    | 2136   | C    | 3.1  |
| 27  | RD    | 99     | ASP  | 3.1  |
| 37  | RR    | 2      | ARG  | 3.1  |
| 38  | RS    | 43     | GLU  | 3.1  |
| 38  | RS    | 111    | GLU  | 3.1  |
| 43  | RX    | 65     | ARG  | 3.1  |
| 48  | R2    | 66     | GLU  | 3.1  |
| 52  | Y6    | 6      | ARG  | 3.1  |
| 3   | XC    | 174    | PRO  | 3.1  |
| 52  | R6    | 16     | CYS  | 3.1  |
| 1   | QA    | 1127   | G    | 3.1  |
| 1   | XA    | 413    | G    | 3.1  |
| 2   | QB    | 5      | ILE  | 3.1  |
| 2   | XB    | 41     | ILE  | 3.1  |
| 17  | QQ    | 32     | TYR  | 3.1  |
| 24  | QX    | 3      | G    | 3.1  |
| 25  | RA    | 1051   | G    | 3.1  |
| 25  | RA    | 1093   | G    | 3.1  |
| 44  | RY    | 44     | ILE  | 3.1  |
| 30  | RG    | 7      | LEU  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | RP    | 35   | HIS  | 3.1  |
| 40  | RU    | 86   | ALA  | 3.1  |
| 9   | QI    | 19   | LEU  | 3.1  |
| 20  | XT    | 72   | LEU  | 3.1  |
| 4   | XD    | 16   | GLY  | 3.1  |
| 4   | QD    | 115  | ARG  | 3.1  |
| 16  | QP    | 71   | ARG  | 3.1  |
| 3   | XC    | 154  | SER  | 3.1  |
| 4   | XD    | 137  | SER  | 3.1  |
| 13  | XM    | 54   | VAL  | 3.1  |
| 13  | QM    | 64   | TRP  | 3.1  |
| 14  | XN    | 17   | LYS  | 3.1  |
| 19  | QS    | 6    | LYS  | 3.1  |
| 20  | QT    | 38   | LYS  | 3.1  |
| 36  | RQ    | 11   | LYS  | 3.1  |
| 38  | YS    | 111  | GLU  | 3.1  |
| 10  | XJ    | 17   | ASP  | 3.1  |
| 25  | YA    | 2114 | A    | 3.1  |
| 39  | RT    | 33   | LYS  | 3.1  |
| 49  | R3    | 17   | LYS  | 3.1  |
| 45  | RZ    | 87   | ASP  | 3.1  |
| 44  | RY    | 55   | TYR  | 3.1  |
| 30  | YG    | 151  | ALA  | 3.0  |
| 31  | RH    | 20   | ALA  | 3.0  |
| 47  | Y1    | 98   | LEU  | 3.0  |
| 14  | QN    | 49   | HIS  | 3.0  |
| 35  | RP    | 81   | GLN  | 3.0  |
| 8   | XH    | 18   | ARG  | 3.0  |
| 25  | RA    | 1062 | G    | 3.0  |
| 32  | YI    | 27   | ARG  | 3.0  |
| 36  | RQ    | 51   | ARG  | 3.0  |
| 40  | RU    | 118  | GLY  | 3.0  |
| 42  | YW    | 92   | ARG  | 3.0  |
| 25  | YA    | 2172 | U    | 3.0  |
| 31  | RH    | 11   | VAL  | 3.0  |
| 36  | YQ    | 104  | PHE  | 3.0  |
| 12  | QL    | 73   | GLU  | 3.0  |
| 32  | YI    | 41   | GLU  | 3.0  |
| 47  | Y1    | 89   | GLU  | 3.0  |
| 4   | XD    | 7    | PRO  | 3.0  |
| 52  | Y6    | 21   | TYR  | 3.0  |
| 17  | QQ    | 31   | LEU  | 3.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 30         | YG           | 133        | LEU         | 3.0         |
| 1          | XA           | 1183       | A           | 3.0         |
| 2          | QB           | 19         | HIS         | 3.0         |
| 19         | XS           | 69         | HIS         | 3.0         |
| 4          | XD           | 159        | ARG         | 3.0         |
| 10         | QJ           | 46         | ARG         | 3.0         |
| 12         | XL           | 89         | ARG         | 3.0         |
| 13         | QM           | 88         | ARG         | 3.0         |
| 15         | QO           | 65         | ARG         | 3.0         |
| 53         | Y7           | 23         | ARG         | 3.0         |
| 55         | R9           | 4          | ARG         | 3.0         |
| 25         | RA           | 1049       | C           | 3.0         |
| 41         | YV           | 42         | GLY         | 3.0         |
| 2          | XB           | 136        | VAL         | 3.0         |
| 35         | RP           | 86         | LYS         | 3.0         |
| 41         | YV           | 37         | VAL         | 3.0         |
| 8          | QH           | 33         | GLU         | 3.0         |
| 27         | YD           | 237        | GLU         | 3.0         |
| 28         | RE           | 73         | GLU         | 3.0         |
| 47         | R1           | 57         | GLU         | 3.0         |
| 30         | YG           | 88         | ILE         | 3.0         |
| 1          | XA           | 1159       | U           | 3.0         |
| 25         | RA           | 2797       | U           | 3.0         |
| 54         | R8           | 37         | SER         | 3.0         |
| 25         | RA           | 1176       | G           | 3.0         |
| 19         | QS           | 16         | LEU         | 3.0         |
| 31         | RH           | 67         | LEU         | 3.0         |
| 45         | YZ           | 183        | LEU         | 3.0         |
| 55         | Y9           | 12         | ASP         | 3.0         |
| 21         | XU           | 6          | ARG         | 3.0         |
| 33         | YN           | 134        | ARG         | 3.0         |
| 14         | XN           | 40         | CYS         | 3.0         |
| 15         | QO           | 51         | HIS         | 3.0         |
| 52         | R6           | 49         | HIS         | 3.0         |
| 4          | XD           | 87         | GLY         | 3.0         |
| 6          | XF           | 11         | ASN         | 3.0         |
| 7          | QG           | 34         | GLY         | 3.0         |
| 30         | RG           | 130        | ASN         | 3.0         |
| 33         | YN           | 81         | GLY         | 3.0         |
| 53         | R7           | 32         | LYS         | 3.0         |
| 25         | YA           | 529        | A           | 3.0         |
| 25         | YA           | 1045       | A           | 3.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | YA    | 2171 | A    | 3.0  |
| 31  | RH    | 169  | VAL  | 3.0  |
| 13  | XM    | 4    | ILE  | 3.0  |
| 25  | RA    | 2164 | C    | 3.0  |
| 25  | RA    | 2474 | C    | 3.0  |
| 26  | RB    | 4    | C    | 3.0  |
| 31  | YH    | 121  | ILE  | 3.0  |
| 3   | QC    | 20   | SER  | 3.0  |
| 10  | QJ    | 8    | LEU  | 3.0  |
| 20  | QT    | 72   | LEU  | 3.0  |
| 29  | RF    | 33   | LEU  | 3.0  |
| 44  | YY    | 17   | SER  | 3.0  |
| 4   | XD    | 111  | ALA  | 3.0  |
| 9   | XI    | 4    | TYR  | 3.0  |
| 13  | QM    | 5    | ALA  | 3.0  |
| 25  | RA    | 9    | U    | 3.0  |
| 9   | XI    | 39   | GLY  | 3.0  |
| 27  | RD    | 100  | GLY  | 3.0  |
| 27  | RD    | 128  | GLY  | 3.0  |
| 36  | YQ    | 15   | GLY  | 3.0  |
| 4   | XD    | 148  | VAL  | 3.0  |
| 12  | XL    | 96   | VAL  | 3.0  |
| 25  | RA    | 1056 | G    | 3.0  |
| 25  | RA    | 1074 | G    | 3.0  |
| 31  | YH    | 125  | VAL  | 3.0  |
| 31  | YH    | 139  | GLN  | 3.0  |
| 51  | Y5    | 45   | VAL  | 3.0  |
| 16  | XP    | 22   | THR  | 3.0  |
| 33  | YN    | 43   | THR  | 3.0  |
| 33  | RN    | 1    | MET  | 3.0  |
| 34  | RO    | 1    | MET  | 3.0  |
| 12  | QL    | 27   | LEU  | 3.0  |
| 17  | QQ    | 89   | LEU  | 3.0  |
| 17  | XQ    | 96   | GLU  | 3.0  |
| 38  | RS    | 8    | GLU  | 3.0  |
| 42  | YW    | 78   | GLU  | 3.0  |
| 44  | RY    | 64   | GLU  | 3.0  |
| 25  | RA    | 2790 | A    | 3.0  |
| 25  | YA    | 2062 | A    | 3.0  |
| 25  | YA    | 2173 | A    | 3.0  |
| 49  | R3    | 41   | PRO  | 3.0  |
| 7   | QG    | 77   | SER  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | QG    | 145  | ALA  | 3.0  |
| 5   | XE    | 61   | TYR  | 3.0  |
| 25  | RA    | 2179 | C    | 3.0  |
| 38  | RS    | 36   | TYR  | 3.0  |
| 8   | QH    | 4    | ASP  | 3.0  |
| 17  | QQ    | 29   | HIS  | 3.0  |
| 19  | QS    | 45   | VAL  | 3.0  |
| 31  | RH    | 161  | GLY  | 3.0  |
| 40  | YU    | 81   | HIS  | 3.0  |
| 44  | RY    | 93   | GLY  | 3.0  |
| 45  | RZ    | 96   | VAL  | 3.0  |
| 45  | YZ    | 147  | GLY  | 3.0  |
| 25  | YA    | 2113 | U    | 3.0  |
| 30  | YG    | 117  | PHE  | 3.0  |
| 7   | QG    | 84   | ASN  | 3.0  |
| 2   | QB    | 42   | ILE  | 3.0  |
| 11  | QK    | 95   | ILE  | 3.0  |
| 32  | RI    | 109  | ILE  | 3.0  |
| 33  | RN    | 28   | THR  | 3.0  |
| 36  | YQ    | 83   | MET  | 3.0  |
| 38  | RS    | 5    | THR  | 3.0  |
| 3   | XC    | 175  | LEU  | 2.9  |
| 9   | QI    | 96   | LEU  | 2.9  |
| 44  | YY    | 50   | ARG  | 2.9  |
| 47  | Y1    | 6    | GLU  | 2.9  |
| 48  | Y2    | 55   | ARG  | 2.9  |
| 51  | R5    | 55   | ARG  | 2.9  |
| 25  | RA    | 1114 | G    | 2.9  |
| 44  | RY    | 54   | LYS  | 2.9  |
| 49  | R3    | 49   | LYS  | 2.9  |
| 1   | XA    | 130  | A    | 2.9  |
| 10  | QJ    | 36   | GLY  | 2.9  |
| 27  | RD    | 34   | VAL  | 2.9  |
| 41  | YV    | 48   | GLY  | 2.9  |
| 52  | R6    | 48   | VAL  | 2.9  |
| 11  | XK    | 81   | ASP  | 2.9  |
| 27  | YD    | 99   | ASP  | 2.9  |
| 2   | XB    | 163  | PHE  | 2.9  |
| 25  | YA    | 2804 | C    | 2.9  |
| 56  | Z8    | 74   | C    | 2.9  |
| 31  | RH    | 4    | ILE  | 2.9  |
| 4   | QD    | 196  | LEU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | XJ    | 48   | THR  | 2.9  |
| 14  | XN    | 29   | ARG  | 2.9  |
| 15  | XO    | 64   | ARG  | 2.9  |
| 30  | RG    | 43   | LEU  | 2.9  |
| 38  | RS    | 32   | LEU  | 2.9  |
| 52  | Y6    | 36   | LEU  | 2.9  |
| 4   | XD    | 136  | PRO  | 2.9  |
| 7   | QG    | 8    | GLU  | 2.9  |
| 21  | XU    | 14   | TRP  | 2.9  |
| 35  | RP    | 72   | PRO  | 2.9  |
| 50  | Y4    | 38   | LYS  | 2.9  |
| 34  | RO    | 41   | ALA  | 2.9  |
| 5   | XE    | 67   | VAL  | 2.9  |
| 6   | XF    | 90   | VAL  | 2.9  |
| 19  | XS    | 38   | SER  | 2.9  |
| 30  | YG    | 149  | VAL  | 2.9  |
| 9   | XI    | 8    | GLY  | 2.9  |
| 25  | RA    | 508  | G    | 2.9  |
| 25  | RA    | 530  | G    | 2.9  |
| 25  | RA    | 2807 | G    | 2.9  |
| 45  | RZ    | 104  | PHE  | 2.9  |
| 40  | YU    | 97   | ASP  | 2.9  |
| 3   | QC    | 124  | ILE  | 2.9  |
| 45  | RZ    | 53   | ILE  | 2.9  |
| 1   | QA    | 1503 | A    | 2.9  |
| 28  | RE    | 37   | ARG  | 2.9  |
| 8   | QH    | 32   | LYS  | 2.9  |
| 20  | QT    | 68   | LYS  | 2.9  |
| 35  | YP    | 14   | LYS  | 2.9  |
| 42  | RW    | 60   | ASN  | 2.9  |
| 1   | XA    | 1039 | C    | 2.9  |
| 10  | XJ    | 26   | ALA  | 2.9  |
| 25  | RA    | 1102 | C    | 2.9  |
| 25  | RA    | 2137 | C    | 2.9  |
| 30  | YG    | 142  | PRO  | 2.9  |
| 33  | RN    | 68   | GLU  | 2.9  |
| 50  | R4    | 11   | PRO  | 2.9  |
| 55  | R9    | 28   | GLU  | 2.9  |
| 25  | RA    | 1066 | U    | 2.9  |
| 25  | RA    | 2172 | U    | 2.9  |
| 30  | RG    | 5    | VAL  | 2.9  |
| 32  | YI    | 107  | VAL  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | QC    | 158  | GLY  | 2.9  |
| 19  | QS    | 10   | PHE  | 2.9  |
| 19  | QS    | 35   | SER  | 2.9  |
| 27  | YD    | 12   | SER  | 2.9  |
| 31  | RH    | 5    | GLY  | 2.9  |
| 4   | QD    | 33   | MET  | 2.9  |
| 6   | QF    | 16   | GLN  | 2.9  |
| 6   | QF    | 89   | MET  | 2.9  |
| 20  | XT    | 84   | LEU  | 2.9  |
| 21  | QU    | 15   | ARG  | 2.9  |
| 27  | RD    | 64   | ILE  | 2.9  |
| 28  | YE    | 37   | ARG  | 2.9  |
| 36  | YQ    | 7    | MET  | 2.9  |
| 39  | YT    | 95   | ARG  | 2.9  |
| 41  | YV    | 38   | LEU  | 2.9  |
| 49  | Y3    | 32   | GLN  | 2.9  |
| 4   | XD    | 102  | ASP  | 2.9  |
| 14  | XN    | 9    | LYS  | 2.9  |
| 32  | RI    | 118  | LYS  | 2.9  |
| 35  | YP    | 64   | LYS  | 2.9  |
| 36  | YQ    | 22   | LYS  | 2.9  |
| 1   | QA    | 630  | G    | 2.9  |
| 9   | QI    | 106  | ALA  | 2.9  |
| 25  | YA    | 10   | G    | 2.9  |
| 25  | YA    | 2894 | G    | 2.9  |
| 30  | YG    | 59   | GLU  | 2.9  |
| 31  | RH    | 21   | PRO  | 2.9  |
| 35  | RP    | 120  | ALA  | 2.9  |
| 38  | YS    | 55   | ALA  | 2.9  |
| 43  | RX    | 38   | GLU  | 2.9  |
| 1   | XA    | 195  | A    | 2.9  |
| 44  | YY    | 79   | CYS  | 2.9  |
| 47  | Y1    | 70   | VAL  | 2.9  |
| 1   | XA    | 1281 | U    | 2.9  |
| 2   | QB    | 72   | GLY  | 2.9  |
| 12  | XL    | 72   | GLY  | 2.9  |
| 31  | RH    | 157  | TYR  | 2.9  |
| 56  | Z6    | 74   | C    | 2.9  |
| 10  | QJ    | 60   | ARG  | 2.9  |
| 28  | YE    | 19   | ARG  | 2.9  |
| 52  | Y6    | 37   | ARG  | 2.9  |
| 14  | XN    | 6    | LEU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | QT    | 104  | LEU  | 2.9  |
| 27  | RD    | 4    | LYS  | 2.9  |
| 50  | Y4    | 60   | GLN  | 2.9  |
| 9   | XI    | 27   | THR  | 2.9  |
| 27  | YD    | 178  | PRO  | 2.9  |
| 29  | RF    | 166  | ALA  | 2.9  |
| 13  | XM    | 35   | GLU  | 2.9  |
| 17  | QQ    | 58   | GLU  | 2.9  |
| 52  | Y6    | 20   | ASN  | 2.9  |
| 28  | RE    | 21   | VAL  | 2.9  |
| 45  | RZ    | 74   | VAL  | 2.9  |
| 5   | XE    | 124  | GLY  | 2.9  |
| 10  | QJ    | 66   | ARG  | 2.9  |
| 31  | YH    | 101  | ARG  | 2.9  |
| 46  | R0    | 11   | ARG  | 2.9  |
| 48  | R2    | 7    | ARG  | 2.9  |
| 1   | XA    | 532  | A    | 2.9  |
| 25  | RA    | 265  | A    | 2.9  |
| 3   | QC    | 196  | LEU  | 2.9  |
| 25  | RA    | 2210 | G    | 2.9  |
| 25  | RA    | 2833 | G    | 2.9  |
| 30  | YG    | 105  | LYS  | 2.9  |
| 28  | RE    | 159  | HIS  | 2.8  |
| 36  | RQ    | 83   | MET  | 2.9  |
| 41  | RV    | 20   | LEU  | 2.9  |
| 45  | RZ    | 70   | LEU  | 2.9  |
| 52  | R6    | 8    | LYS  | 2.9  |
| 31  | YH    | 38   | SER  | 2.8  |
| 45  | RZ    | 166  | SER  | 2.8  |
| 29  | RF    | 171  | PRO  | 2.8  |
| 30  | YG    | 50   | ALA  | 2.8  |
| 35  | RP    | 103  | ALA  | 2.8  |
| 43  | YX    | 6    | ASP  | 2.8  |
| 12  | QL    | 127  | GLU  | 2.8  |
| 28  | YE    | 143  | ASN  | 2.8  |
| 45  | RZ    | 71   | VAL  | 2.8  |
| 4   | QD    | 3    | ARG  | 2.8  |
| 27  | RD    | 262  | ARG  | 2.8  |
| 11  | XK    | 127  | LYS  | 2.8  |
| 3   | QC    | 39   | ILE  | 2.8  |
| 4   | XD    | 38   | TYR  | 2.8  |
| 10  | XJ    | 88   | LEU  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | YS    | 109  | GLY  | 2.8  |
| 13  | XM    | 9    | ILE  | 2.8  |
| 29  | RF    | 28   | ILE  | 2.8  |
| 30  | YG    | 77   | ILE  | 2.8  |
| 19  | XS    | 14   | HIS  | 2.8  |
| 28  | RE    | 132  | HIS  | 2.8  |
| 25  | RA    | 1088 | A    | 2.8  |
| 25  | RA    | 1177 | A    | 2.8  |
| 25  | RA    | 2170 | A    | 2.8  |
| 41  | RV    | 73   | SER  | 2.8  |
| 45  | YZ    | 149  | SER  | 2.8  |
| 28  | YE    | 204  | ALA  | 2.8  |
| 1   | QA    | 413  | G    | 2.8  |
| 1   | QA    | 1002 | G    | 2.8  |
| 26  | YB    | 1    | U    | 2.8  |
| 28  | YE    | 62   | PRO  | 2.8  |
| 54  | R8    | 53   | PRO  | 2.8  |
| 1   | QA    | 1284 | C    | 2.8  |
| 4   | XD    | 163  | GLU  | 2.8  |
| 5   | QE    | 116  | THR  | 2.8  |
| 17  | QQ    | 49   | GLU  | 2.8  |
| 20  | QT    | 83   | ARG  | 2.8  |
| 25  | RA    | 2804 | C    | 2.8  |
| 34  | YO    | 54   | GLU  | 2.8  |
| 45  | YZ    | 145  | GLU  | 2.8  |
| 48  | Y2    | 51   | ARG  | 2.8  |
| 12  | QL    | 17   | LYS  | 2.8  |
| 2   | QB    | 17   | PHE  | 2.8  |
| 29  | RF    | 134  | GLY  | 2.8  |
| 30  | YG    | 3    | LEU  | 2.8  |
| 40  | YU    | 118  | GLY  | 2.8  |
| 42  | YW    | 91   | GLY  | 2.8  |
| 45  | YZ    | 150  | LEU  | 2.8  |
| 9   | QI    | 4    | TYR  | 2.8  |
| 9   | QI    | 125  | TYR  | 2.8  |
| 46  | Y0    | 17   | GLN  | 2.8  |
| 9   | XI    | 15   | ALA  | 2.8  |
| 14  | XN    | 5    | ALA  | 2.8  |
| 27  | RD    | 12   | SER  | 2.8  |
| 30  | RG    | 46   | ALA  | 2.8  |
| 38  | RS    | 50   | SER  | 2.8  |
| 28  | RE    | 58   | ARG  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | RR    | 68   | ARG  | 2.8  |
| 12  | QL    | 23   | LYS  | 2.8  |
| 27  | YD    | 26   | LYS  | 2.8  |
| 30  | RG    | 59   | GLU  | 2.8  |
| 30  | RG    | 168  | GLU  | 2.8  |
| 31  | YH    | 137  | ASP  | 2.8  |
| 33  | RN    | 2    | LYS  | 2.8  |
| 25  | YA    | 2799 | A    | 2.8  |
| 1   | XA    | 1240 | U    | 2.8  |
| 1   | XA    | 1450 | U    | 2.8  |
| 2   | QB    | 11   | LEU  | 2.8  |
| 2   | QB    | 215  | LEU  | 2.8  |
| 27  | RD    | 70   | TRP  | 2.8  |
| 28  | YE    | 78   | LEU  | 2.8  |
| 13  | QM    | 24   | GLY  | 2.8  |
| 30  | YG    | 85   | GLY  | 2.8  |
| 44  | RY    | 43   | ASN  | 2.8  |
| 54  | Y8    | 41   | ILE  | 2.8  |
| 1   | QA    | 1129 | C    | 2.8  |
| 1   | QA    | 1321 | C    | 2.8  |
| 1   | QA    | 1397 | C    | 2.8  |
| 14  | QN    | 34   | TYR  | 2.8  |
| 25  | RA    | 2803 | C    | 2.8  |
| 25  | YA    | 2151 | G    | 2.8  |
| 26  | YB    | 108  | C    | 2.8  |
| 7   | XG    | 117  | ALA  | 2.8  |
| 30  | RG    | 110  | ALA  | 2.8  |
| 44  | RY    | 48   | ALA  | 2.8  |
| 6   | XF    | 2    | ARG  | 2.8  |
| 39  | RT    | 112  | ARG  | 2.8  |
| 47  | Y1    | 21   | ARG  | 2.8  |
| 52  | R6    | 19   | ARG  | 2.8  |
| 9   | QI    | 53   | VAL  | 2.8  |
| 29  | RF    | 174  | VAL  | 2.8  |
| 31  | YH    | 63   | SER  | 2.8  |
| 50  | Y4    | 35   | VAL  | 2.8  |
| 2   | QB    | 168  | THR  | 2.8  |
| 3   | XC    | 52   | LEU  | 2.8  |
| 30  | YG    | 62   | LEU  | 2.8  |
| 45  | RZ    | 170  | THR  | 2.8  |
| 14  | QN    | 37   | PHE  | 2.8  |
| 36  | RQ    | 66   | ILE  | 2.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 44         | YY           | 44         | ILE         | 2.8         |
| 49         | R3           | 18         | ASP         | 2.8         |
| 50         | R4           | 31         | ILE         | 2.8         |
| 52         | Y6           | 26         | ASN         | 2.8         |
| 1          | QA           | 1126       | U           | 2.8         |
| 5          | XE           | 133        | TYR         | 2.8         |
| 3          | QC           | 190        | ARG         | 2.8         |
| 31         | RH           | 6          | ARG         | 2.8         |
| 55         | Y9           | 18         | ARG         | 2.8         |
| 1          | XA           | 1129       | C           | 2.8         |
| 27         | YD           | 208        | LYS         | 2.8         |
| 38         | RS           | 33         | LYS         | 2.8         |
| 38         | YS           | 59         | LYS         | 2.8         |
| 44         | RY           | 46         | LYS         | 2.8         |
| 52         | R6           | 38         | LYS         | 2.8         |
| 1          | XA           | 220        | G           | 2.8         |
| 25         | RA           | 2190       | G           | 2.8         |
| 25         | YA           | 508        | G           | 2.8         |
| 25         | YA           | 2802       | G           | 2.8         |
| 30         | RG           | 70         | VAL         | 2.8         |
| 31         | YH           | 45         | VAL         | 2.8         |
| 3          | XC           | 91         | LEU         | 2.8         |
| 44         | RY           | 17         | SER         | 2.8         |
| 44         | YY           | 90         | LEU         | 2.8         |
| 2          | QB           | 211        | ILE         | 2.8         |
| 13         | XM           | 43         | THR         | 2.8         |
| 30         | RG           | 54         | GLU         | 2.8         |
| 38         | YS           | 64         | GLU         | 2.8         |
| 54         | Y8           | 54         | GLU         | 2.8         |
| 44         | RY           | 61         | ILE         | 2.8         |
| 27         | YD           | 16         | MET         | 2.7         |
| 30         | RG           | 129        | GLY         | 2.7         |
| 31         | RH           | 100        | GLY         | 2.7         |
| 42         | YW           | 60         | ASN         | 2.7         |
| 7          | XG           | 115        | ARG         | 2.7         |
| 19         | QS           | 47         | HIS         | 2.7         |
| 37         | RR           | 8          | ARG         | 2.7         |
| 2          | QB           | 132        | LYS         | 2.7         |
| 2          | XB           | 13         | ALA         | 2.7         |
| 2          | XB           | 22         | LYS         | 2.7         |
| 9          | QI           | 45         | ALA         | 2.7         |
| 12         | XL           | 91         | LYS         | 2.7         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 27  | RD    | 35     | LYS  | 2.7  |
| 30  | YG    | 158    | ALA  | 2.7  |
| 47  | R1    | 78     | LYS  | 2.7  |
| 50  | Y4    | 28     | LYS  | 2.7  |
| 9   | XI    | 28     | VAL  | 2.7  |
| 25  | YA    | 2629   | A    | 2.7  |
| 25  | YA    | 2897   | U    | 2.7  |
| 31  | RH    | 52     | VAL  | 2.7  |
| 35  | RP    | 38     | GLN  | 2.7  |
| 21  | XU    | 23     | PRO  | 2.7  |
| 4   | XD    | 120    | LEU  | 2.7  |
| 14  | QN    | 47     | LEU  | 2.7  |
| 1   | QA    | 1066   | C    | 2.7  |
| 1   | XA    | 345    | C    | 2.7  |
| 10  | QJ    | 35     | SER  | 2.7  |
| 12  | XL    | 73     | GLU  | 2.7  |
| 14  | QN    | 42     | ILE  | 2.7  |
| 9   | QI    | 64     | THR  | 2.7  |
| 25  | RA    | 974(A) | C    | 2.7  |
| 25  | RA    | 1075   | C    | 2.7  |
| 28  | YE    | 73     | GLU  | 2.7  |
| 31  | YH    | 86     | GLU  | 2.7  |
| 36  | RQ    | 104    | PHE  | 2.7  |
| 27  | RD    | 238    | GLY  | 2.7  |
| 1   | QA    | 351    | G    | 2.7  |
| 13  | XM    | 11     | ARG  | 2.7  |
| 37  | YR    | 2      | ARG  | 2.7  |
| 10  | XJ    | 69     | ASN  | 2.7  |
| 33  | RN    | 70     | LYS  | 2.7  |
| 52  | Y6    | 29     | ASN  | 2.7  |
| 2   | XB    | 237    | ALA  | 2.7  |
| 4   | XD    | 164    | ALA  | 2.7  |
| 10  | QJ    | 26     | ALA  | 2.7  |
| 28  | RE    | 131    | ALA  | 2.7  |
| 47  | R1    | 30     | VAL  | 2.7  |
| 7   | QG    | 38     | LEU  | 2.7  |
| 21  | QU    | 23     | PRO  | 2.7  |
| 27  | RD    | 149    | PRO  | 2.7  |
| 29  | RF    | 181    | LEU  | 2.7  |
| 30  | YG    | 32     | PRO  | 2.7  |
| 30  | YG    | 179    | PRO  | 2.7  |
| 34  | RO    | 72     | PRO  | 2.7  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | QA    | 1281   | U    | 2.7  |
| 19  | QS    | 40     | ILE  | 2.7  |
| 25  | YA    | 271(C) | U    | 2.7  |
| 34  | RO    | 2      | ILE  | 2.7  |
| 2   | QB    | 170    | GLU  | 2.7  |
| 28  | RE    | 40     | GLU  | 2.7  |
| 34  | RO    | 9      | GLU  | 2.7  |
| 34  | RO    | 54     | GLU  | 2.7  |
| 45  | YZ    | 181    | GLU  | 2.7  |
| 1   | QA    | 1280   | A    | 2.7  |
| 1   | XA    | 1032   | A    | 2.7  |
| 4   | XD    | 152    | SER  | 2.7  |
| 25  | RA    | 2126   | A    | 2.7  |
| 44  | YY    | 83     | THR  | 2.7  |
| 45  | RZ    | 69     | THR  | 2.7  |
| 10  | XJ    | 66     | ARG  | 2.7  |
| 38  | RS    | 13     | ARG  | 2.7  |
| 21  | XU    | 25     | LYS  | 2.7  |
| 28  | RE    | 118    | LYS  | 2.7  |
| 35  | YP    | 86     | LYS  | 2.7  |
| 38  | YS    | 33     | LYS  | 2.7  |
| 25  | RA    | 1104   | C    | 2.7  |
| 25  | RA    | 2791   | C    | 2.7  |
| 40  | YU    | 91     | ASP  | 2.7  |
| 10  | QJ    | 68     | HIS  | 2.7  |
| 39  | RT    | 104    | ASN  | 2.7  |
| 4   | XD    | 133    | VAL  | 2.7  |
| 41  | RV    | 5      | VAL  | 2.7  |
| 49  | R3    | 47     | VAL  | 2.7  |
| 29  | RF    | 176    | LEU  | 2.7  |
| 35  | RP    | 123    | LEU  | 2.7  |
| 3   | XC    | 162    | GLN  | 2.7  |
| 12  | QL    | 48     | PRO  | 2.7  |
| 16  | QP    | 76     | GLN  | 2.7  |
| 25  | YA    | 892    | G    | 2.7  |
| 27  | YD    | 241    | PRO  | 2.7  |
| 28  | RE    | 62     | PRO  | 2.7  |
| 3   | QC    | 186    | PHE  | 2.7  |
| 11  | QK    | 29     | ILE  | 2.7  |
| 49  | R3    | 48     | GLU  | 2.7  |
| 3   | XC    | 190    | ARG  | 2.7  |
| 9   | XI    | 93     | ARG  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | QK    | 31   | THR  | 2.7  |
| 11  | XK    | 96   | ARG  | 2.7  |
| 17  | XQ    | 91   | ARG  | 2.7  |
| 29  | YF    | 117  | ARG  | 2.7  |
| 3   | QC    | 167  | TRP  | 2.7  |
| 51  | R5    | 10   | LYS  | 2.7  |
| 25  | RA    | 1729 | A    | 2.7  |
| 25  | RA    | 2176 | A    | 2.7  |
| 25  | YA    | 2176 | A    | 2.7  |
| 51  | Y5    | 17   | ASP  | 2.7  |
| 28  | RE    | 75   | VAL  | 2.7  |
| 36  | RQ    | 79   | LEU  | 2.7  |
| 41  | RV    | 72   | VAL  | 2.7  |
| 11  | XK    | 117  | ASN  | 2.7  |
| 1   | XA    | 163  | C    | 2.7  |
| 3   | XC    | 7    | PRO  | 2.7  |
| 7   | QG    | 27   | ILE  | 2.7  |
| 10  | QJ    | 91   | PRO  | 2.7  |
| 17  | XQ    | 36   | ILE  | 2.7  |
| 32  | RI    | 137  | PRO  | 2.7  |
| 20  | XT    | 85   | MET  | 2.7  |
| 5   | XE    | 25   | ARG  | 2.7  |
| 7   | XG    | 41   | ARG  | 2.7  |
| 15  | QO    | 64   | ARG  | 2.7  |
| 17  | XQ    | 75   | ARG  | 2.7  |
| 21  | QU    | 6    | ARG  | 2.7  |
| 36  | RQ    | 10   | ARG  | 2.7  |
| 9   | QI    | 2    | GLU  | 2.7  |
| 15  | QO    | 61   | GLY  | 2.7  |
| 28  | YE    | 194  | GLY  | 2.7  |
| 31  | RH    | 86   | GLU  | 2.7  |
| 35  | YP    | 107  | LYS  | 2.7  |
| 50  | Y4    | 64   | GLY  | 2.7  |
| 1   | QA    | 993  | G    | 2.7  |
| 1   | QA    | 1053 | G    | 2.7  |
| 1   | XA    | 346  | G    | 2.7  |
| 22  | QV    | 6    | G    | 2.7  |
| 41  | RV    | 56   | SER  | 2.7  |
| 45  | YZ    | 142  | SER  | 2.7  |
| 15  | QO    | 30   | ALA  | 2.7  |
| 29  | YF    | 128  | ALA  | 2.7  |
| 30  | YG    | 46   | ALA  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | YP    | 12   | ALA  | 2.7  |
| 1   | QA    | 1125 | U    | 2.7  |
| 6   | XF    | 40   | VAL  | 2.7  |
| 11  | XK    | 25   | TYR  | 2.7  |
| 14  | QN    | 6    | LEU  | 2.7  |
| 25  | RA    | 2895 | U    | 2.7  |
| 31  | YH    | 19   | VAL  | 2.7  |
| 4   | XD    | 53   | ASP  | 2.7  |
| 27  | RD    | 66   | ASP  | 2.7  |
| 40  | RU    | 56   | ASP  | 2.7  |
| 41  | RV    | 26   | ASP  | 2.7  |
| 30  | RG    | 108  | ASN  | 2.7  |
| 54  | R8    | 33   | ASN  | 2.7  |
| 1   | QA    | 974  | A    | 2.6  |
| 5   | QE    | 66   | MET  | 2.6  |
| 7   | QG    | 11   | GLN  | 2.6  |
| 25  | RA    | 2117 | A    | 2.6  |
| 25  | YA    | 646  | A    | 2.6  |
| 28  | RE    | 56   | PRO  | 2.6  |
| 39  | RT    | 42   | ILE  | 2.6  |
| 50  | R4    | 5    | ILE  | 2.6  |
| 55  | R9    | 26   | ILE  | 2.6  |
| 13  | XM    | 104  | ARG  | 2.6  |
| 36  | YQ    | 5    | ARG  | 2.6  |
| 38  | RS    | 87   | PHE  | 2.6  |
| 42  | RW    | 92   | ARG  | 2.6  |
| 8   | XH    | 46   | LYS  | 2.6  |
| 12  | XL    | 13   | LYS  | 2.6  |
| 40  | YU    | 13   | LYS  | 2.6  |
| 51  | Y5    | 3    | LYS  | 2.6  |
| 2   | QB    | 143  | GLU  | 2.6  |
| 14  | QN    | 55   | GLY  | 2.6  |
| 27  | YD    | 181  | GLU  | 2.6  |
| 40  | YU    | 89   | GLU  | 2.6  |
| 47  | R1    | 55   | GLY  | 2.6  |
| 25  | YA    | 2177 | C    | 2.6  |
| 35  | RP    | 32   | THR  | 2.6  |
| 12  | QL    | 128  | ALA  | 2.6  |
| 27  | YD    | 240  | ALA  | 2.6  |
| 32  | YI    | 65   | ALA  | 2.6  |
| 48  | R2    | 4    | SER  | 2.6  |
| 50  | R4    | 33   | VAL  | 2.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 36  | RQ    | 123    | HIS  | 2.6  |
| 45  | RZ    | 32     | HIS  | 2.6  |
| 46  | Y0    | 3      | HIS  | 2.6  |
| 1   | QA    | 1131   | G    | 2.6  |
| 4   | XD    | 118    | ARG  | 2.6  |
| 13  | QM    | 10     | PRO  | 2.6  |
| 16  | XP    | 25     | ARG  | 2.6  |
| 20  | XT    | 8      | ARG  | 2.6  |
| 25  | RA    | 654(A) | G    | 2.6  |
| 25  | RA    | 1107   | G    | 2.6  |
| 31  | RH    | 162    | ILE  | 2.6  |
| 39  | RT    | 124    | ASP  | 2.6  |
| 45  | RZ    | 77     | ASP  | 2.6  |
| 4   | QD    | 160    | GLN  | 2.6  |
| 4   | QD    | 161    | ASN  | 2.6  |
| 9   | QI    | 70     | LYS  | 2.6  |
| 10  | XJ    | 63     | PHE  | 2.6  |
| 29  | RF    | 66     | PRO  | 2.6  |
| 27  | YD    | 164    | GLN  | 2.6  |
| 30  | RG    | 75     | LYS  | 2.6  |
| 30  | RG    | 112    | PRO  | 2.6  |
| 34  | YO    | 5      | GLN  | 2.6  |
| 36  | RQ    | 89     | ASN  | 2.6  |
| 1   | XA    | 632    | A    | 2.6  |
| 1   | XA    | 1286   | A    | 2.6  |
| 42  | RW    | 78     | GLU  | 2.6  |
| 45  | RZ    | 84     | GLU  | 2.6  |
| 10  | QJ    | 81     | THR  | 2.6  |
| 14  | QN    | 13     | THR  | 2.6  |
| 39  | RT    | 60     | THR  | 2.6  |
| 4   | QD    | 162    | LEU  | 2.6  |
| 29  | RF    | 11     | VAL  | 2.6  |
| 29  | RF    | 132    | VAL  | 2.6  |
| 31  | RH    | 87     | LEU  | 2.6  |
| 4   | QD    | 152    | SER  | 2.6  |
| 19  | XS    | 35     | SER  | 2.6  |
| 25  | YA    | 277    | C    | 2.6  |
| 36  | RQ    | 137    | TYR  | 2.6  |
| 50  | Y4    | 43     | TYR  | 2.6  |
| 15  | XO    | 65     | ARG  | 2.6  |
| 27  | RD    | 268    | ARG  | 2.6  |
| 28  | RE    | 76     | ARG  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | RP    | 16   | ARG  | 2.6  |
| 16  | XP    | 1    | MET  | 2.6  |
| 52  | R6    | 25   | LYS  | 2.6  |
| 52  | R6    | 53   | LYS  | 2.6  |
| 52  | Y6    | 53   | LYS  | 2.6  |
| 39  | RT    | 22   | PHE  | 2.6  |
| 6   | XF    | 74   | ASP  | 2.6  |
| 20  | QT    | 18   | GLN  | 2.6  |
| 27  | RD    | 44   | ASN  | 2.6  |
| 35  | YP    | 68   | GLN  | 2.6  |
| 5   | XE    | 22   | GLY  | 2.6  |
| 25  | YA    | 2167 | U    | 2.6  |
| 32  | RI    | 41   | GLU  | 2.6  |
| 39  | RT    | 73   | GLU  | 2.6  |
| 45  | RZ    | 138  | GLU  | 2.6  |
| 45  | YZ    | 162  | GLU  | 2.6  |
| 1   | QA    | 64   | G    | 2.6  |
| 25  | YA    | 1087 | G    | 2.6  |
| 25  | YA    | 1678 | G    | 2.6  |
| 2   | XB    | 11   | LEU  | 2.6  |
| 5   | QE    | 94   | ALA  | 2.6  |
| 11  | XK    | 87   | THR  | 2.6  |
| 13  | XM    | 37   | THR  | 2.6  |
| 29  | YF    | 24   | LEU  | 2.6  |
| 30  | YG    | 165  | THR  | 2.6  |
| 34  | RO    | 25   | LEU  | 2.6  |
| 38  | RS    | 54   | LEU  | 2.6  |
| 44  | YY    | 67   | LEU  | 2.6  |
| 53  | Y7    | 45   | ALA  | 2.6  |
| 14  | QN    | 50   | LYS  | 2.6  |
| 16  | QP    | 5    | ARG  | 2.6  |
| 25  | RA    | 896  | A    | 2.6  |
| 55  | Y9    | 2    | LYS  | 2.6  |
| 2   | XB    | 148  | TYR  | 2.6  |
| 19  | QS    | 44   | MET  | 2.6  |
| 9   | XI    | 49   | PRO  | 2.6  |
| 15  | QO    | 75   | PRO  | 2.6  |
| 19  | QS    | 2    | PRO  | 2.6  |
| 2   | XB    | 95   | GLN  | 2.6  |
| 37  | RR    | 69   | ASP  | 2.6  |
| 41  | YV    | 80   | GLN  | 2.6  |
| 13  | QM    | 62   | ASN  | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 30         | YG           | 129        | GLY         | 2.6         |
| 32         | RI           | 84         | GLY         | 2.6         |
| 33         | RN           | 64         | GLY         | 2.6         |
| 38         | RS           | 109        | GLY         | 2.6         |
| 55         | Y9           | 29         | ASN         | 2.6         |
| 8          | QH           | 99         | GLU         | 2.6         |
| 47         | R1           | 72         | GLU         | 2.6         |
| 47         | Y1           | 27         | GLU         | 2.6         |
| 47         | Y1           | 80         | LEU         | 2.6         |
| 7          | QG           | 75         | VAL         | 2.6         |
| 8          | QH           | 3          | THR         | 2.6         |
| 9          | QI           | 15         | ALA         | 2.6         |
| 13         | QM           | 45         | VAL         | 2.6         |
| 18         | QR           | 22         | VAL         | 2.6         |
| 20         | QT           | 66         | ALA         | 2.6         |
| 31         | RH           | 50         | VAL         | 2.6         |
| 2          | QB           | 139        | LYS         | 2.6         |
| 10         | QJ           | 70         | ARG         | 2.6         |
| 12         | QL           | 13         | LYS         | 2.6         |
| 17         | QQ           | 3          | LYS         | 2.6         |
| 20         | QT           | 25         | ARG         | 2.6         |
| 25         | RA           | 2689       | U           | 2.6         |
| 28         | RE           | 154        | LYS         | 2.6         |
| 30         | YG           | 8          | LYS         | 2.6         |
| 55         | Y9           | 22         | ARG         | 2.6         |
| 4          | XD           | 26         | CYS         | 2.6         |
| 14         | XN           | 7          | ILE         | 2.6         |
| 36         | RQ           | 7          | MET         | 2.6         |
| 1          | QA           | 1443       | G           | 2.6         |
| 16         | QP           | 41         | PRO         | 2.6         |
| 35         | YP           | 56         | SER         | 2.6         |
| 38         | RS           | 27         | SER         | 2.6         |
| 50         | Y4           | 41         | PRO         | 2.6         |
| 1          | QA           | 465        | A           | 2.6         |
| 25         | RA           | 1095       | A           | 2.6         |
| 28         | RE           | 190        | GLY         | 2.6         |
| 30         | RG           | 4          | ASP         | 2.6         |
| 30         | RG           | 150        | ASP         | 2.6         |
| 45         | RZ           | 115        | GLY         | 2.6         |
| 13         | QM           | 12         | ASN         | 2.6         |
| 4          | QD           | 194        | LEU         | 2.6         |
| 7          | QG           | 12         | LEU         | 2.6         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | QM    | 70   | LEU  | 2.6  |
| 33  | YN    | 33   | LEU  | 2.6  |
| 39  | RT    | 105  | LEU  | 2.6  |
| 41  | YV    | 18   | LEU  | 2.6  |
| 43  | RX    | 92   | LEU  | 2.6  |
| 1   | QA    | 934  | C    | 2.6  |
| 6   | QF    | 66   | GLU  | 2.6  |
| 14  | XN    | 33   | VAL  | 2.6  |
| 24  | QX    | 5    | C    | 2.6  |
| 27  | RD    | 30   | GLU  | 2.6  |
| 48  | Y2    | 5    | GLU  | 2.6  |
| 2   | QB    | 186  | ALA  | 2.6  |
| 4   | QD    | 48   | ALA  | 2.6  |
| 4   | XD    | 30   | LYS  | 2.6  |
| 7   | QG    | 108  | ALA  | 2.6  |
| 9   | QI    | 41   | VAL  | 2.6  |
| 11  | QK    | 89   | ALA  | 2.6  |
| 14  | QN    | 58   | LYS  | 2.6  |
| 27  | RD    | 38   | LYS  | 2.6  |
| 27  | RD    | 263  | ARG  | 2.6  |
| 30  | YG    | 118  | ARG  | 2.6  |
| 36  | RQ    | 28   | ALA  | 2.6  |
| 2   | QB    | 6    | THR  | 2.6  |
| 10  | QJ    | 92   | THR  | 2.6  |
| 29  | RF    | 65   | TRP  | 2.5  |
| 30  | RG    | 161  | THR  | 2.6  |
| 8   | XH    | 109  | ILE  | 2.5  |
| 17  | QQ    | 65   | ILE  | 2.5  |
| 1   | QA    | 723  | U    | 2.5  |
| 9   | XI    | 62   | TYR  | 2.5  |
| 25  | RA    | 1113 | U    | 2.5  |
| 34  | RO    | 93   | PRO  | 2.5  |
| 4   | QD    | 83   | SER  | 2.5  |
| 38  | YS    | 27   | SER  | 2.5  |
| 20  | QT    | 102  | GLY  | 2.5  |
| 27  | YD    | 234  | GLY  | 2.5  |
| 28  | RE    | 186  | GLY  | 2.5  |
| 28  | YE    | 54   | GLN  | 2.5  |
| 35  | RP    | 11   | GLY  | 2.5  |
| 41  | YV    | 40   | LEU  | 2.5  |
| 3   | QC    | 30   | ARG  | 2.5  |
| 8   | QH    | 18   | ARG  | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 21         | XU           | 9          | ARG         | 2.5         |
| 1          | XA           | 1151       | A           | 2.5         |
| 4          | QD           | 156        | GLU         | 2.5         |
| 8          | QH           | 28         | ALA         | 2.5         |
| 8          | QH           | 132        | GLU         | 2.5         |
| 13         | XM           | 32         | GLU         | 2.5         |
| 17         | QQ           | 85         | VAL         | 2.5         |
| 25         | YA           | 1089       | G           | 2.5         |
| 27         | RD           | 5          | LYS         | 2.5         |
| 27         | RD           | 239        | ARG         | 2.5         |
| 28         | RE           | 121        | ASN         | 2.5         |
| 28         | YE           | 55         | ASN         | 2.5         |
| 30         | YG           | 113        | ARG         | 2.5         |
| 31         | YH           | 58         | GLU         | 2.5         |
| 34         | RO           | 45         | GLU         | 2.5         |
| 35         | RP           | 12         | ALA         | 2.5         |
| 36         | YQ           | 48         | GLU         | 2.5         |
| 36         | YQ           | 90         | VAL         | 2.5         |
| 53         | R7           | 8          | ASN         | 2.5         |
| 25         | RA           | 654        | A           | 2.5         |
| 25         | YA           | 6          | A           | 2.5         |
| 40         | YU           | 96         | ALA         | 2.5         |
| 2          | QB           | 214        | ILE         | 2.5         |
| 10         | QJ           | 15         | THR         | 2.5         |
| 30         | RG           | 114        | ILE         | 2.5         |
| 11         | QK           | 20         | TYR         | 2.5         |
| 31         | YH           | 10         | PRO         | 2.5         |
| 4          | QD           | 26         | CYS         | 2.5         |
| 10         | QJ           | 19         | SER         | 2.5         |
| 1          | XA           | 5          | U           | 2.5         |
| 1          | XA           | 65         | U           | 2.5         |
| 15         | QO           | 71         | GLN         | 2.5         |
| 19         | QS           | 56         | GLN         | 2.5         |
| 28         | RE           | 88         | GLY         | 2.5         |
| 50         | R4           | 17         | GLY         | 2.5         |
| 9          | QI           | 10         | ARG         | 2.5         |
| 13         | XM           | 3          | ARG         | 2.5         |
| 19         | QS           | 3          | ARG         | 2.5         |
| 20         | XT           | 34         | LYS         | 2.5         |
| 39         | YT           | 112        | ARG         | 2.5         |
| 47         | R1           | 26         | ARG         | 2.5         |
| 14         | QN           | 56         | VAL         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 19         | XS           | 13         | ASP         | 2.5         |
| 29         | YF           | 161        | GLU         | 2.5         |
| 31         | RH           | 18         | GLU         | 2.5         |
| 31         | YH           | 81         | GLU         | 2.5         |
| 43         | YX           | 75         | ASP         | 2.5         |
| 2          | QB           | 201        | ILE         | 2.5         |
| 13         | QM           | 37         | THR         | 2.5         |
| 50         | Y4           | 27         | THR         | 2.5         |
| 16         | XP           | 9          | PHE         | 2.5         |
| 28         | YE           | 67         | PHE         | 2.5         |
| 38         | RS           | 29         | PHE         | 2.5         |
| 1          | XA           | 172        | A           | 2.5         |
| 1          | QA           | 438        | G           | 2.5         |
| 1          | XA           | 1453       | G           | 2.5         |
| 22         | XV           | 53         | G           | 2.5         |
| 25         | RA           | 1888       | G           | 2.5         |
| 5          | XE           | 49         | PRO         | 2.5         |
| 10         | XJ           | 91         | PRO         | 2.5         |
| 31         | RH           | 164        | TYR         | 2.5         |
| 1          | QA           | 979        | C           | 2.5         |
| 1          | QA           | 1234       | C           | 2.5         |
| 1          | XA           | 221        | C           | 2.5         |
| 1          | XA           | 1054       | C           | 2.5         |
| 7          | QG           | 3          | ARG         | 2.5         |
| 13         | XM           | 121        | LYS         | 2.5         |
| 17         | XQ           | 81         | ARG         | 2.5         |
| 27         | YD           | 239        | ARG         | 2.5         |
| 29         | RF           | 192        | LEU         | 2.5         |
| 25         | RA           | 1052       | C           | 2.5         |
| 25         | YA           | 2136       | C           | 2.5         |
| 30         | RG           | 128        | ARG         | 2.5         |
| 35         | RP           | 65         | ARG         | 2.5         |
| 35         | RP           | 116        | GLY         | 2.5         |
| 43         | YX           | 65         | ARG         | 2.5         |
| 51         | Y5           | 37         | LYS         | 2.5         |
| 54         | R8           | 36         | LYS         | 2.5         |
| 17         | XQ           | 35         | VAL         | 2.5         |
| 31         | RH           | 131        | VAL         | 2.5         |
| 36         | RQ           | 90         | VAL         | 2.5         |
| 44         | RY           | 98         | VAL         | 2.5         |
| 45         | YZ           | 111        | VAL         | 2.5         |
| 2          | QB           | 77         | ALA         | 2.5         |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 13  | QM    | 75      | ALA  | 2.5  |
| 32  | RI    | 53      | ALA  | 2.5  |
| 1   | XA    | 173     | U    | 2.5  |
| 1   | XA    | 841     | U    | 2.5  |
| 2   | QB    | 231     | GLU  | 2.5  |
| 25  | RA    | 2808    | U    | 2.5  |
| 26  | RB    | 1       | U    | 2.5  |
| 30  | RG    | 167     | GLU  | 2.5  |
| 43  | RX    | 44      | GLU  | 2.5  |
| 54  | R8    | 56      | GLU  | 2.5  |
| 20  | XT    | 64      | ASP  | 2.5  |
| 40  | YU    | 94      | ASN  | 2.5  |
| 35  | RP    | 1       | MET  | 2.5  |
| 36  | YQ    | 1       | MET  | 2.5  |
| 54  | R8    | 25      | MET  | 2.5  |
| 33  | YN    | 63      | THR  | 2.5  |
| 34  | RO    | 99      | PHE  | 2.5  |
| 3   | XC    | 150     | LYS  | 2.5  |
| 4   | QD    | 27      | TYR  | 2.5  |
| 10  | XJ    | 68      | HIS  | 2.5  |
| 10  | XJ    | 90      | LEU  | 2.5  |
| 14  | XN    | 34      | TYR  | 2.5  |
| 19  | QS    | 52      | TYR  | 2.5  |
| 30  | RG    | 21      | ARG  | 2.5  |
| 44  | RY    | 6       | HIS  | 2.5  |
| 44  | RY    | 34      | LYS  | 2.5  |
| 47  | R1    | 69      | LYS  | 2.5  |
| 47  | R1    | 76      | ARG  | 2.5  |
| 50  | Y4    | 71      | ARG  | 2.5  |
| 55  | Y9    | 19      | ARG  | 2.5  |
| 1   | QA    | 975     | A    | 2.5  |
| 1   | QA    | 1110    | A    | 2.5  |
| 1   | QA    | 1363    | A    | 2.5  |
| 5   | QE    | 22      | GLY  | 2.5  |
| 19  | XS    | 72      | GLY  | 2.5  |
| 25  | RA    | 278     | A    | 2.5  |
| 25  | YA    | 654(U)  | A    | 2.5  |
| 25  | YA    | 1444(A) | A    | 2.5  |
| 32  | RI    | 16      | GLY  | 2.5  |
| 2   | XB    | 165     | VAL  | 2.5  |
| 27  | YD    | 46      | GLN  | 2.5  |
| 35  | YP    | 70      | GLN  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | R3    | 32   | GLN  | 2.5  |
| 1   | XA    | 190  | G    | 2.5  |
| 2   | QB    | 34   | ALA  | 2.5  |
| 3   | XC    | 169  | ALA  | 2.5  |
| 11  | QK    | 19   | ALA  | 2.5  |
| 25  | RA    | 615  | G    | 2.5  |
| 25  | RA    | 859  | G    | 2.5  |
| 25  | RA    | 2160 | G    | 2.5  |
| 44  | RY    | 70   | SER  | 2.5  |
| 2   | XB    | 4    | GLU  | 2.5  |
| 30  | RG    | 45   | GLU  | 2.5  |
| 30  | YG    | 140  | ILE  | 2.5  |
| 31  | YH    | 34   | GLU  | 2.5  |
| 48  | R2    | 11   | GLU  | 2.5  |
| 50  | Y4    | 5    | ILE  | 2.5  |
| 25  | RA    | 1100 | C    | 2.5  |
| 25  | RA    | 2402 | C    | 2.5  |
| 51  | R5    | 48   | GLU  | 2.5  |
| 9   | XI    | 101  | PHE  | 2.5  |
| 11  | QK    | 81   | ASP  | 2.5  |
| 50  | R4    | 51   | ASP  | 2.5  |
| 2   | XB    | 190  | THR  | 2.5  |
| 11  | QK    | 42   | TRP  | 2.5  |
| 25  | RA    | 1372 | U    | 2.5  |
| 20  | XT    | 14   | LYS  | 2.5  |
| 27  | RD    | 68   | LYS  | 2.5  |
| 27  | YD    | 4    | LYS  | 2.5  |
| 33  | RN    | 65   | LYS  | 2.5  |
| 30  | YG    | 7    | LEU  | 2.5  |
| 30  | YG    | 33   | ARG  | 2.5  |
| 52  | R6    | 17   | LYS  | 2.5  |
| 2   | QB    | 196  | LEU  | 2.5  |
| 5   | QE    | 70   | PRO  | 2.5  |
| 9   | QI    | 102  | LEU  | 2.5  |
| 10  | QJ    | 39   | PRO  | 2.5  |
| 17  | XQ    | 98   | LEU  | 2.5  |
| 31  | RH    | 88   | LEU  | 2.5  |
| 35  | RP    | 135  | LEU  | 2.5  |
| 35  | YP    | 99   | LEU  | 2.5  |
| 39  | RT    | 68   | TYR  | 2.5  |
| 7   | XG    | 81   | GLY  | 2.5  |
| 6   | QF    | 91   | VAL  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | QE    | 104  | ALA  | 2.4  |
| 47  | Y1    | 77   | ALA  | 2.4  |
| 2   | XB    | 80   | ILE  | 2.4  |
| 9   | XI    | 77   | ILE  | 2.4  |
| 13  | XM    | 67   | GLU  | 2.4  |
| 20  | QT    | 60   | GLU  | 2.4  |
| 25  | RA    | 2062 | A    | 2.4  |
| 25  | YA    | 1096 | A    | 2.4  |
| 25  | YA    | 1177 | A    | 2.4  |
| 25  | YA    | 2169 | A    | 2.4  |
| 52  | Y6    | 35   | GLU  | 2.4  |
| 2   | XB    | 175  | ARG  | 2.4  |
| 2   | XB    | 198  | ASP  | 2.4  |
| 2   | XB    | 220  | ASP  | 2.4  |
| 9   | QI    | 11   | LYS  | 2.4  |
| 10  | QJ    | 17   | ASP  | 2.4  |
| 16  | XP    | 42   | ARG  | 2.4  |
| 29  | RF    | 133  | ASN  | 2.4  |
| 30  | YG    | 10   | LYS  | 2.4  |
| 30  | YG    | 36   | LYS  | 2.4  |
| 30  | YG    | 40   | ASN  | 2.4  |
| 32  | RI    | 113  | ARG  | 2.4  |
| 35  | YP    | 87   | ASP  | 2.4  |
| 39  | RT    | 137  | LYS  | 2.4  |
| 39  | YT    | 93   | ARG  | 2.4  |
| 40  | RU    | 61   | TRP  | 2.4  |
| 40  | RU    | 92   | ARG  | 2.4  |
| 1   | QA    | 266  | G    | 2.4  |
| 11  | QK    | 41   | THR  | 2.4  |
| 1   | QA    | 1149 | C    | 2.4  |
| 1   | XA    | 388  | G    | 2.4  |
| 4   | QD    | 97   | LEU  | 2.4  |
| 13  | QM    | 43   | THR  | 2.4  |
| 48  | Y2    | 52   | ASP  | 2.4  |
| 25  | RA    | 889  | C    | 2.4  |
| 25  | RA    | 2108 | C    | 2.4  |
| 25  | RA    | 2490 | G    | 2.4  |
| 25  | RA    | 2795 | G    | 2.4  |
| 25  | YA    | 2124 | G    | 2.4  |
| 44  | YY    | 14   | LEU  | 2.4  |
| 27  | RD    | 11   | PRO  | 2.4  |
| 32  | YI    | 134  | PRO  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | QH    | 94  | TYR  | 2.4  |
| 55  | Y9    | 24  | TYR  | 2.4  |
| 3   | QC    | 148 | GLY  | 2.4  |
| 4   | XD    | 104 | VAL  | 2.4  |
| 28  | YE    | 65  | GLY  | 2.4  |
| 29  | YF    | 121 | GLY  | 2.4  |
| 31  | RH    | 43  | VAL  | 2.4  |
| 31  | YH    | 144 | VAL  | 2.4  |
| 39  | YT    | 56  | GLY  | 2.4  |
| 50  | R4    | 35  | VAL  | 2.4  |
| 11  | XK    | 128 | ALA  | 2.4  |
| 27  | YD    | 253 | GLN  | 2.4  |
| 30  | RG    | 171 | ALA  | 2.4  |
| 40  | RU    | 116 | ALA  | 2.4  |
| 47  | R1    | 47  | GLN  | 2.4  |
| 54  | R8    | 55  | ALA  | 2.4  |
| 19  | XS    | 40  | ILE  | 2.4  |
| 4   | QD    | 28  | SER  | 2.4  |
| 5   | XE    | 50  | GLU  | 2.4  |
| 6   | QF    | 17  | SER  | 2.4  |
| 27  | YD    | 162 | SER  | 2.4  |
| 2   | XB    | 21  | ARG  | 2.4  |
| 2   | XB    | 36  | ARG  | 2.4  |
| 4   | QD    | 139 | ARG  | 2.4  |
| 8   | XH    | 85  | ARG  | 2.4  |
| 10  | XJ    | 7   | LYS  | 2.4  |
| 21  | QU    | 25  | LYS  | 2.4  |
| 30  | YG    | 115 | ARG  | 2.4  |
| 48  | Y2    | 49  | LYS  | 2.4  |
| 4   | XD    | 135 | LEU  | 2.4  |
| 44  | RY    | 90  | LEU  | 2.4  |
| 1   | QA    | 994 | A    | 2.4  |
| 2   | XB    | 6   | THR  | 2.4  |
| 15  | QO    | 25  | THR  | 2.4  |
| 19  | QS    | 53  | ASN  | 2.4  |
| 27  | YD    | 44  | ASN  | 2.4  |
| 16  | XP    | 41  | PRO  | 2.4  |
| 25  | RA    | 653 | A    | 2.4  |
| 11  | QK    | 80  | VAL  | 2.4  |
| 30  | RG    | 109 | VAL  | 2.4  |
| 30  | YG    | 25  | TYR  | 2.4  |
| 33  | YN    | 9   | VAL  | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 35  | RP    | 128    | HIS  | 2.4  |
| 36  | RQ    | 88     | GLY  | 2.4  |
| 50  | R4    | 40     | HIS  | 2.4  |
| 50  | Y4    | 21     | VAL  | 2.4  |
| 1   | QA    | 701    | C    | 2.4  |
| 1   | XA    | 980    | C    | 2.4  |
| 3   | XC    | 71     | ALA  | 2.4  |
| 4   | XD    | 32     | ALA  | 2.4  |
| 9   | XI    | 119    | ALA  | 2.4  |
| 1   | QA    | 485    | G    | 2.4  |
| 1   | QA    | 1272   | G    | 2.4  |
| 7   | XG    | 110    | GLN  | 2.4  |
| 10  | QJ    | 82     | ILE  | 2.4  |
| 13  | XM    | 118    | ALA  | 2.4  |
| 10  | XJ    | 84     | GLN  | 2.4  |
| 16  | XP    | 76     | GLN  | 2.4  |
| 22  | XV    | 5      | G    | 2.4  |
| 25  | RA    | 2112   | G    | 2.4  |
| 25  | RA    | 2162   | G    | 2.4  |
| 25  | RA    | 2168   | G    | 2.4  |
| 25  | RA    | 2211   | G    | 2.4  |
| 25  | YA    | 270(L) | U    | 2.4  |
| 25  | YA    | 1101   | U    | 2.4  |
| 25  | YA    | 1534   | G    | 2.4  |
| 27  | RD    | 116    | GLN  | 2.4  |
| 3   | XC    | 156    | ARG  | 2.4  |
| 9   | QI    | 121    | ARG  | 2.4  |
| 14  | QN    | 57     | ARG  | 2.4  |
| 16  | QP    | 75     | ARG  | 2.4  |
| 28  | RE    | 57     | LYS  | 2.4  |
| 30  | RG    | 30     | GLU  | 2.4  |
| 36  | RQ    | 29     | PHE  | 2.4  |
| 40  | YU    | 112    | ARG  | 2.4  |
| 50  | Y4    | 42     | PHE  | 2.4  |
| 8   | QH    | 87     | SER  | 2.4  |
| 12  | QL    | 10     | LEU  | 2.4  |
| 12  | XL    | 27     | LEU  | 2.4  |
| 3   | QC    | 7      | PRO  | 2.4  |
| 44  | YY    | 77     | PRO  | 2.4  |
| 4   | QD    | 203    | VAL  | 2.4  |
| 4   | XD    | 88     | VAL  | 2.4  |
| 6   | QF    | 90     | VAL  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | RF    | 23   | ASP  | 2.4  |
| 41  | RV    | 37   | VAL  | 2.4  |
| 50  | R4    | 50   | VAL  | 2.4  |
| 55  | Y9    | 23   | VAL  | 2.4  |
| 8   | QH    | 66   | GLY  | 2.4  |
| 8   | QH    | 130  | GLY  | 2.4  |
| 12  | XL    | 95   | GLY  | 2.4  |
| 27  | YD    | 190  | TYR  | 2.4  |
| 28  | YE    | 66   | HIS  | 2.4  |
| 2   | XB    | 39   | ILE  | 2.4  |
| 4   | QD    | 5    | ILE  | 2.4  |
| 14  | XN    | 30   | ALA  | 2.4  |
| 20  | QT    | 41   | ILE  | 2.4  |
| 30  | RG    | 52   | ILE  | 2.4  |
| 30  | YG    | 56   | ALA  | 2.4  |
| 44  | YY    | 75   | ILE  | 2.4  |
| 45  | YZ    | 109  | ALA  | 2.4  |
| 25  | RA    | 2134 | A    | 2.4  |
| 25  | YA    | 276  | A    | 2.4  |
| 25  | YA    | 899  | A    | 2.4  |
| 25  | YA    | 1069 | A    | 2.4  |
| 7   | XG    | 35   | LYS  | 2.4  |
| 37  | RR    | 71   | GLN  | 2.4  |
| 39  | YT    | 90   | GLN  | 2.4  |
| 50  | R4    | 60   | GLN  | 2.4  |
| 52  | Y6    | 19   | ARG  | 2.4  |
| 27  | YD    | 269  | PHE  | 2.4  |
| 31  | RH    | 109  | PHE  | 2.4  |
| 3   | QC    | 87   | LEU  | 2.4  |
| 4   | XD    | 162  | LEU  | 2.4  |
| 6   | QF    | 78   | GLU  | 2.4  |
| 17  | XQ    | 61   | GLU  | 2.4  |
| 30  | RG    | 18   | GLU  | 2.4  |
| 31  | YH    | 71   | LEU  | 2.4  |
| 36  | YQ    | 34   | LEU  | 2.4  |
| 41  | RV    | 94   | LEU  | 2.4  |
| 44  | YY    | 29   | GLU  | 2.4  |
| 48  | R2    | 5    | GLU  | 2.4  |
| 27  | YD    | 266  | SER  | 2.4  |
| 33  | YN    | 76   | SER  | 2.4  |
| 25  | RA    | 101  | G    | 2.4  |
| 25  | RA    | 275  | G    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | YA    | 2793 | G    | 2.4  |
| 7   | QG    | 156  | TRP  | 2.4  |
| 2   | XB    | 239  | VAL  | 2.4  |
| 12  | XL    | 125  | PRO  | 2.4  |
| 31  | RH    | 141  | VAL  | 2.4  |
| 31  | YH    | 35   | VAL  | 2.4  |
| 34  | RO    | 102  | VAL  | 2.4  |
| 4   | QD    | 53   | ASP  | 2.4  |
| 13  | QM    | 95   | GLY  | 2.4  |
| 33  | YN    | 127  | ASP  | 2.4  |
| 35  | YP    | 142  | GLY  | 2.4  |
| 50  | Y4    | 40   | HIS  | 2.4  |
| 7   | XG    | 30   | ILE  | 2.4  |
| 45  | RZ    | 124  | ILE  | 2.4  |
| 48  | Y2    | 50   | ILE  | 2.4  |
| 55  | R9    | 17   | ILE  | 2.4  |
| 20  | QT    | 65   | LYS  | 2.4  |
| 44  | YY    | 46   | LYS  | 2.4  |
| 20  | QT    | 85   | MET  | 2.4  |
| 28  | RE    | 19   | ARG  | 2.4  |
| 45  | RZ    | 20   | ARG  | 2.4  |
| 51  | Y5    | 55   | ARG  | 2.4  |
| 7   | QG    | 110  | GLN  | 2.4  |
| 11  | QK    | 99   | GLN  | 2.4  |
| 20  | QT    | 42   | GLN  | 2.4  |
| 45  | RZ    | 73   | GLN  | 2.4  |
| 47  | Y1    | 19   | GLN  | 2.4  |
| 9   | XI    | 59   | PHE  | 2.4  |
| 32  | YI    | 116  | LEU  | 2.4  |
| 17  | XQ    | 58   | GLU  | 2.4  |
| 43  | YX    | 23   | GLU  | 2.4  |
| 44  | RY    | 29   | GLU  | 2.4  |
| 4   | QD    | 71   | SER  | 2.4  |
| 47  | R1    | 86   | SER  | 2.4  |
| 1   | XA    | 723  | U    | 2.4  |
| 10  | QJ    | 101  | VAL  | 2.4  |
| 25  | RA    | 1101 | U    | 2.4  |
| 35  | RP    | 19   | VAL  | 2.4  |
| 45  | RZ    | 56   | VAL  | 2.4  |
| 50  | R4    | 7    | PRO  | 2.4  |
| 25  | RA    | 1076 | C    | 2.3  |
| 25  | RA    | 1109 | C    | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | XD    | 167  | GLY  | 2.3  |
| 35  | YP    | 24   | GLY  | 2.3  |
| 51  | R5    | 11   | THR  | 2.3  |
| 54  | Y8    | 27   | THR  | 2.3  |
| 2   | XB    | 31   | TYR  | 2.3  |
| 9   | QI    | 63   | ILE  | 2.3  |
| 20  | XT    | 65   | LYS  | 2.3  |
| 38  | RS    | 11   | LYS  | 2.3  |
| 44  | YY    | 33   | LYS  | 2.3  |
| 45  | YZ    | 75   | ASN  | 2.3  |
| 9   | XI    | 5    | TYR  | 2.3  |
| 10  | XJ    | 9    | ARG  | 2.3  |
| 11  | XK    | 126  | ARG  | 2.3  |
| 13  | QM    | 108  | ARG  | 2.3  |
| 16  | XP    | 8    | ARG  | 2.3  |
| 20  | QT    | 64   | ASP  | 2.3  |
| 30  | YG    | 98   | ARG  | 2.3  |
| 39  | YT    | 51   | ARG  | 2.3  |
| 44  | RY    | 11   | ASP  | 2.3  |
| 2   | QB    | 101  | MET  | 2.3  |
| 28  | RE    | 168  | MET  | 2.3  |
| 25  | RA    | 1055 | G    | 2.3  |
| 25  | RA    | 2120 | G    | 2.3  |
| 25  | YA    | 1063 | G    | 2.3  |
| 25  | YA    | 2156 | G    | 2.3  |
| 25  | YA    | 2160 | G    | 2.3  |
| 25  | YA    | 2190 | G    | 2.3  |
| 2   | XB    | 187  | LEU  | 2.3  |
| 4   | QD    | 110  | PHE  | 2.3  |
| 10  | QJ    | 90   | LEU  | 2.3  |
| 27  | RD    | 257  | LEU  | 2.3  |
| 29  | RF    | 27   | GLU  | 2.3  |
| 30  | RG    | 104  | GLU  | 2.3  |
| 35  | YP    | 117  | GLU  | 2.3  |
| 5   | QE    | 82   | VAL  | 2.3  |
| 30  | YG    | 38   | VAL  | 2.3  |
| 1   | XA    | 452  | A    | 2.3  |
| 2   | QB    | 18   | GLY  | 2.3  |
| 3   | XC    | 147  | LYS  | 2.3  |
| 5   | QE    | 103  | GLY  | 2.3  |
| 17  | XQ    | 17   | LYS  | 2.3  |
| 20  | XT    | 74   | LYS  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 6    | A    | 2.3  |
| 25  | RA    | 1086 | A    | 2.3  |
| 25  | RA    | 2114 | A    | 2.3  |
| 25  | YA    | 1057 | A    | 2.3  |
| 25  | YA    | 1729 | A    | 2.3  |
| 29  | YF    | 137  | LYS  | 2.3  |
| 30  | YG    | 182  | LYS  | 2.3  |
| 28  | YE    | 111  | ARG  | 2.3  |
| 29  | YF    | 82   | ILE  | 2.3  |
| 31  | RH    | 59   | ARG  | 2.3  |
| 35  | YP    | 116  | GLY  | 2.3  |
| 36  | RQ    | 100  | GLY  | 2.3  |
| 46  | R0    | 22   | GLY  | 2.3  |
| 50  | Y4    | 8    | LYS  | 2.3  |
| 2   | QB    | 88   | ALA  | 2.3  |
| 2   | XB    | 173  | ALA  | 2.3  |
| 2   | XB    | 222  | ILE  | 2.3  |
| 4   | XD    | 9    | CYS  | 2.3  |
| 10  | QJ    | 23   | ILE  | 2.3  |
| 50  | Y4    | 52   | THR  | 2.3  |
| 31  | RH    | 111  | HIS  | 2.3  |
| 40  | RU    | 81   | HIS  | 2.3  |
| 1   | XA    | 1025 | U    | 2.3  |
| 4   | QD    | 38   | TYR  | 2.3  |
| 4   | QD    | 77   | ASN  | 2.3  |
| 5   | QE    | 130  | ASN  | 2.3  |
| 17  | XQ    | 42   | TYR  | 2.3  |
| 25  | YA    | 2122 | U    | 2.3  |
| 35  | RP    | 84   | ASN  | 2.3  |
| 40  | RU    | 66   | ASN  | 2.3  |
| 33  | YN    | 50   | ASP  | 2.3  |
| 2   | QB    | 238  | LEU  | 2.3  |
| 2   | QB    | 240  | GLN  | 2.3  |
| 9   | XI    | 18   | PHE  | 2.3  |
| 15  | QO    | 15   | PHE  | 2.3  |
| 28  | RE    | 51   | PHE  | 2.3  |
| 35  | RP    | 148  | LEU  | 2.3  |
| 35  | YP    | 106  | LEU  | 2.3  |
| 36  | RQ    | 2    | LEU  | 2.3  |
| 55  | Y9    | 36   | GLN  | 2.3  |
| 9   | QI    | 12   | GLU  | 2.3  |
| 14  | XN    | 8    | GLU  | 2.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 43         | YX           | 44         | GLU         | 2.3         |
| 1          | QA           | 1160       | G           | 2.3         |
| 1          | XA           | 1127       | G           | 2.3         |
| 6          | XF           | 37         | VAL         | 2.3         |
| 9          | QI           | 109        | VAL         | 2.3         |
| 25         | RA           | 2149       | G           | 2.3         |
| 25         | YA           | 1899       | G           | 2.3         |
| 36         | RQ           | 35         | VAL         | 2.3         |
| 45         | RZ           | 174        | VAL         | 2.3         |
| 50         | R4           | 10         | VAL         | 2.3         |
| 55         | R9           | 3          | VAL         | 2.3         |
| 4          | QD           | 46         | LYS         | 2.3         |
| 21         | QU           | 3          | LYS         | 2.3         |
| 34         | RO           | 31         | LYS         | 2.3         |
| 36         | YQ           | 18         | LYS         | 2.3         |
| 41         | RV           | 76         | LYS         | 2.3         |
| 47         | Y1           | 69         | LYS         | 2.3         |
| 9          | QI           | 123        | PRO         | 2.3         |
| 9          | XI           | 128        | ARG         | 2.3         |
| 10         | XJ           | 51         | ARG         | 2.3         |
| 17         | XQ           | 63         | ARG         | 2.3         |
| 20         | QT           | 23         | ARG         | 2.3         |
| 45         | RZ           | 167        | PRO         | 2.3         |
| 2          | XB           | 38         | GLY         | 2.3         |
| 5          | QE           | 39         | GLY         | 2.3         |
| 3          | XC           | 165        | THR         | 2.3         |
| 4          | XD           | 127        | THR         | 2.3         |
| 11         | QK           | 43         | SER         | 2.3         |
| 13         | QM           | 112        | GLY         | 2.3         |
| 16         | XP           | 69         | THR         | 2.3         |
| 17         | QQ           | 39         | SER         | 2.3         |
| 29         | RF           | 206        | ILE         | 2.3         |
| 31         | RH           | 142        | GLY         | 2.3         |
| 45         | YZ           | 114        | GLY         | 2.3         |
| 29         | YF           | 177        | ALA         | 2.3         |
| 38         | RS           | 95         | HIS         | 2.3         |
| 50         | R4           | 6          | HIS         | 2.3         |
| 4          | QD           | 4          | TYR         | 2.3         |
| 21         | XU           | 18         | TYR         | 2.3         |
| 51         | R5           | 33         | CYS         | 2.3         |
| 51         | Y5           | 33         | CYS         | 2.3         |
| 6          | QF           | 79         | LEU         | 2.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | XJ    | 40   | LEU  | 2.3  |
| 13  | XM    | 106  | ASN  | 2.3  |
| 16  | XP    | 6    | LEU  | 2.3  |
| 30  | YG    | 106  | LEU  | 2.3  |
| 32  | YI    | 6    | LEU  | 2.3  |
| 35  | YP    | 148  | LEU  | 2.3  |
| 1   | XA    | 974  | A    | 2.3  |
| 1   | XA    | 1130 | A    | 2.3  |
| 25  | RA    | 1847 | A    | 2.3  |
| 25  | YA    | 1460 | A    | 2.3  |
| 29  | RF    | 202  | PHE  | 2.3  |
| 11  | QK    | 36   | ASP  | 2.3  |
| 1   | QA    | 208  | U    | 2.3  |
| 7   | QG    | 13   | GLN  | 2.3  |
| 19  | QS    | 43   | GLU  | 2.3  |
| 48  | Y2    | 66   | GLU  | 2.3  |
| 54  | R8    | 54   | GLU  | 2.3  |
| 1   | QA    | 1019 | C    | 2.3  |
| 4   | QD    | 30   | LYS  | 2.3  |
| 25  | YA    | 2175 | C    | 2.3  |
| 26  | RB    | 28   | C    | 2.3  |
| 30  | YG    | 109  | VAL  | 2.3  |
| 36  | RQ    | 27   | VAL  | 2.3  |
| 39  | RT    | 98   | LYS  | 2.3  |
| 45  | YZ    | 105  | VAL  | 2.3  |
| 7   | XG    | 78   | ARG  | 2.3  |
| 13  | XM    | 99   | ARG  | 2.3  |
| 21  | QU    | 7    | ARG  | 2.3  |
| 34  | RO    | 97   | ARG  | 2.3  |
| 43  | RX    | 73   | ARG  | 2.3  |
| 3   | QC    | 9    | GLY  | 2.3  |
| 4   | XD    | 23   | GLY  | 2.3  |
| 16  | XP    | 19   | ILE  | 2.3  |
| 35  | YP    | 63   | PRO  | 2.3  |
| 47  | R1    | 84   | GLY  | 2.3  |
| 30  | YG    | 73   | ALA  | 2.3  |
| 34  | YO    | 30   | ALA  | 2.3  |
| 2   | XB    | 101  | MET  | 2.3  |
| 30  | RG    | 165  | THR  | 2.3  |
| 30  | YG    | 148  | MET  | 2.3  |
| 19  | XS    | 47   | HIS  | 2.3  |
| 20  | XT    | 70   | SER  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | QT    | 24   | LEU  | 2.3  |
| 31  | RH    | 158  | HIS  | 2.3  |
| 1   | QA    | 1177 | G    | 2.3  |
| 7   | QG    | 154  | TYR  | 2.3  |
| 9   | XI    | 33   | PHE  | 2.3  |
| 25  | RA    | 916  | G    | 2.3  |
| 25  | RA    | 1332 | G    | 2.3  |
| 25  | YA    | 101  | G    | 2.3  |
| 25  | YA    | 1888 | G    | 2.3  |
| 25  | YA    | 2149 | G    | 2.3  |
| 6   | QF    | 13   | ASN  | 2.3  |
| 12  | QL    | 49   | ASN  | 2.3  |
| 29  | RF    | 169  | ASN  | 2.3  |
| 30  | RG    | 40   | ASN  | 2.3  |
| 45  | RZ    | 75   | ASN  | 2.3  |
| 33  | RN    | 133  | GLN  | 2.3  |
| 45  | YZ    | 63   | ASP  | 2.3  |
| 17  | QQ    | 87   | LYS  | 2.3  |
| 20  | QT    | 21   | LYS  | 2.3  |
| 27  | YD    | 5    | LYS  | 2.3  |
| 31  | RH    | 85   | LYS  | 2.3  |
| 41  | YV    | 6    | LYS  | 2.3  |
| 41  | YV    | 19   | LYS  | 2.3  |
| 54  | R8    | 59   | LYS  | 2.3  |
| 2   | QB    | 93   | VAL  | 2.3  |
| 3   | QC    | 156  | ARG  | 2.3  |
| 8   | QH    | 93   | VAL  | 2.3  |
| 8   | XH    | 93   | VAL  | 2.3  |
| 11  | XK    | 14   | VAL  | 2.3  |
| 14  | XN    | 23   | ARG  | 2.3  |
| 16  | XP    | 75   | ARG  | 2.3  |
| 18  | XR    | 42   | ARG  | 2.3  |
| 21  | QU    | 22   | ARG  | 2.3  |
| 25  | YA    | 330  | A    | 2.3  |
| 26  | RB    | 52   | A    | 2.3  |
| 28  | RE    | 165  | VAL  | 2.3  |
| 34  | RO    | 98   | VAL  | 2.3  |
| 37  | RR    | 33   | ARG  | 2.3  |
| 1   | QA    | 65   | U    | 2.3  |
| 26  | RB    | 41   | U    | 2.3  |
| 35  | RP    | 75   | ILE  | 2.3  |
| 44  | RY    | 53   | PRO  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | QG    | 152  | ALA  | 2.3  |
| 11  | QK    | 90   | GLY  | 2.3  |
| 13  | XM    | 75   | ALA  | 2.3  |
| 16  | QP    | 30   | GLY  | 2.3  |
| 30  | RG    | 163  | ALA  | 2.3  |
| 33  | RN    | 36   | GLY  | 2.3  |
| 35  | YP    | 143  | GLY  | 2.3  |
| 41  | YV    | 27   | ALA  | 2.3  |
| 44  | YY    | 18   | GLY  | 2.3  |
| 10  | XJ    | 86   | MET  | 2.3  |
| 23  | QY    | 28   | C    | 2.3  |
| 25  | RA    | 915  | C    | 2.3  |
| 25  | RA    | 1072 | C    | 2.3  |
| 25  | YA    | 1075 | C    | 2.3  |
| 33  | RN    | 13   | TRP  | 2.3  |
| 13  | XM    | 103  | THR  | 2.3  |
| 16  | QP    | 6    | LEU  | 2.3  |
| 27  | RD    | 27   | THR  | 2.3  |
| 27  | RD    | 37   | LEU  | 2.3  |
| 28  | RE    | 38   | THR  | 2.3  |
| 31  | YH    | 105  | LEU  | 2.3  |
| 53  | R7    | 43   | THR  | 2.3  |
| 2   | QB    | 152  | PHE  | 2.3  |
| 12  | XL    | 32   | PHE  | 2.3  |
| 33  | YN    | 4    | TYR  | 2.3  |
| 12  | QL    | 21   | LYS  | 2.3  |
| 33  | RN    | 37   | LYS  | 2.3  |
| 40  | RU    | 19   | LYS  | 2.3  |
| 44  | YY    | 92   | ASN  | 2.3  |
| 3   | QC    | 179  | ARG  | 2.3  |
| 8   | QH    | 30   | ARG  | 2.3  |
| 9   | QI    | 93   | ARG  | 2.3  |
| 13  | QM    | 99   | ARG  | 2.3  |
| 14  | XN    | 35   | ARG  | 2.3  |
| 27  | RD    | 176  | ARG  | 2.3  |
| 33  | YN    | 114  | ARG  | 2.3  |
| 48  | R2    | 46   | GLN  | 2.3  |
| 53  | R7    | 33   | ARG  | 2.3  |
| 9   | QI    | 75   | ASP  | 2.3  |
| 30  | YG    | 159  | VAL  | 2.3  |
| 37  | RR    | 49   | ASP  | 2.3  |
| 39  | RT    | 122  | ASP  | 2.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 39  | YT    | 87     | ASP  | 2.3  |
| 6   | QF    | 95     | GLU  | 2.2  |
| 10  | QJ    | 61     | GLU  | 2.2  |
| 12  | XL    | 127    | GLU  | 2.2  |
| 13  | QM    | 61     | GLU  | 2.2  |
| 1   | QA    | 306    | G    | 2.2  |
| 1   | QA    | 1036   | G    | 2.2  |
| 1   | QA    | 1202   | G    | 2.2  |
| 25  | RA    | 10     | G    | 2.2  |
| 25  | RA    | 1534   | G    | 2.2  |
| 25  | RA    | 2805   | G    | 2.2  |
| 25  | YA    | 654(A) | G    | 2.2  |
| 25  | YA    | 2162   | G    | 2.2  |
| 50  | Y4    | 14     | ILE  | 2.2  |
| 6   | XF    | 56     | PRO  | 2.2  |
| 17  | QQ    | 15     | MET  | 2.2  |
| 20  | XT    | 56     | MET  | 2.2  |
| 21  | QU    | 11     | GLY  | 2.2  |
| 27  | YD    | 108    | PRO  | 2.2  |
| 30  | RG    | 32     | PRO  | 2.2  |
| 32  | RI    | 83     | ALA  | 2.2  |
| 44  | RY    | 59     | GLY  | 2.2  |
| 1   | XA    | 1157   | A    | 2.2  |
| 8   | QH    | 2      | LEU  | 2.2  |
| 19  | XS    | 15     | LEU  | 2.2  |
| 19  | XS    | 71     | LEU  | 2.2  |
| 25  | RA    | 2132   | U    | 2.2  |
| 2   | QB    | 181    | PHE  | 2.2  |
| 14  | XN    | 13     | THR  | 2.2  |
| 16  | QP    | 13     | HIS  | 2.2  |
| 17  | QQ    | 27     | PHE  | 2.2  |
| 30  | RG    | 125    | PHE  | 2.2  |
| 35  | RP    | 30     | THR  | 2.2  |
| 4   | XD    | 4      | TYR  | 2.2  |
| 10  | QJ    | 99     | LYS  | 2.2  |
| 13  | XM    | 111    | LYS  | 2.2  |
| 14  | QN    | 9      | LYS  | 2.2  |
| 16  | XP    | 11     | SER  | 2.2  |
| 19  | QS    | 61     | TYR  | 2.2  |
| 28  | YE    | 69     | LYS  | 2.2  |
| 29  | RF    | 104    | LYS  | 2.2  |
| 30  | RG    | 182    | LYS  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | YG    | 75   | LYS  | 2.2  |
| 39  | YT    | 12   | SER  | 2.2  |
| 40  | RU    | 77   | SER  | 2.2  |
| 43  | YX    | 72   | LYS  | 2.2  |
| 47  | Y1    | 17   | SER  | 2.2  |
| 1   | QA    | 88   | C    | 2.2  |
| 1   | QA    | 1051 | C    | 2.2  |
| 1   | XA    | 1137 | C    | 2.2  |
| 4   | QD    | 49   | ARG  | 2.2  |
| 7   | QG    | 41   | ARG  | 2.2  |
| 23  | QY    | 34   | C    | 2.2  |
| 25  | YA    | 2111 | C    | 2.2  |
| 38  | RS    | 17   | ARG  | 2.2  |
| 9   | QI    | 14   | VAL  | 2.2  |
| 31  | RH    | 144  | VAL  | 2.2  |
| 12  | XL    | 92   | ASP  | 2.2  |
| 12  | XL    | 112  | ASP  | 2.2  |
| 28  | RE    | 127  | ASP  | 2.2  |
| 30  | YG    | 167  | GLU  | 2.2  |
| 33  | YN    | 96   | GLU  | 2.2  |
| 35  | RP    | 136  | GLU  | 2.2  |
| 2   | XB    | 108  | ILE  | 2.2  |
| 5   | QE    | 109  | ILE  | 2.2  |
| 4   | XD    | 155  | LEU  | 2.2  |
| 5   | QE    | 119  | LEU  | 2.2  |
| 5   | QE    | 138  | ALA  | 2.2  |
| 8   | XH    | 55   | GLY  | 2.2  |
| 13  | XM    | 18   | ALA  | 2.2  |
| 21  | XU    | 11   | GLY  | 2.2  |
| 27  | RD    | 119  | ALA  | 2.2  |
| 31  | RH    | 33   | LEU  | 2.2  |
| 31  | YH    | 87   | LEU  | 2.2  |
| 35  | YP    | 150  | ALA  | 2.2  |
| 40  | YU    | 73   | GLY  | 2.2  |
| 44  | RY    | 5    | MET  | 2.2  |
| 50  | R4    | 41   | PRO  | 2.2  |
| 1   | QA    | 1034 | G    | 2.2  |
| 2   | QB    | 133  | LYS  | 2.2  |
| 4   | XD    | 89   | THR  | 2.2  |
| 12  | XL    | 28   | LYS  | 2.2  |
| 30  | YG    | 141  | PHE  | 2.2  |
| 24  | XX    | 3    | G    | 2.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 24  | XX    | 6     | G    | 2.2  |
| 25  | YA    | 275   | G    | 2.2  |
| 25  | YA    | 2893  | G    | 2.2  |
| 33  | YN    | 7     | LYS  | 2.2  |
| 35  | RP    | 27    | HIS  | 2.2  |
| 1   | QA    | 1450  | U    | 2.2  |
| 4   | QD    | 122   | ARG  | 2.2  |
| 8   | XH    | 84    | ARG  | 2.2  |
| 10  | XJ    | 28    | ARG  | 2.2  |
| 18  | QR    | 54    | ARG  | 2.2  |
| 22  | XV    | 17(A) | U    | 2.2  |
| 25  | RA    | 1083  | U    | 2.2  |
| 25  | YA    | 2150  | U    | 2.2  |
| 27  | RD    | 217   | ARG  | 2.2  |
| 28  | YE    | 151   | TYR  | 2.2  |
| 29  | RF    | 44    | ARG  | 2.2  |
| 48  | Y2    | 7     | ARG  | 2.2  |
| 50  | R4    | 43    | TYR  | 2.2  |
| 55  | R9    | 18    | ARG  | 2.2  |
| 1   | QA    | 1041  | A    | 2.2  |
| 5   | QE    | 34    | VAL  | 2.2  |
| 9   | QI    | 44    | VAL  | 2.2  |
| 16  | QP    | 2     | VAL  | 2.2  |
| 29  | RF    | 37    | VAL  | 2.2  |
| 38  | RS    | 49    | VAL  | 2.2  |
| 4   | QD    | 74    | GLN  | 2.2  |
| 8   | XH    | 35    | ILE  | 2.2  |
| 10  | QJ    | 96    | ILE  | 2.2  |
| 10  | XJ    | 23    | ILE  | 2.2  |
| 13  | XM    | 50    | GLU  | 2.2  |
| 30  | YG    | 143   | GLU  | 2.2  |
| 36  | RQ    | 38    | GLU  | 2.2  |
| 40  | RU    | 88    | ILE  | 2.2  |
| 44  | YY    | 96    | ILE  | 2.2  |
| 50  | Y4    | 39    | CYS  | 2.2  |
| 1   | XA    | 307   | C    | 2.2  |
| 2   | QB    | 221   | LEU  | 2.2  |
| 3   | XC    | 204   | LEU  | 2.2  |
| 8   | XH    | 54    | ASP  | 2.2  |
| 11  | QK    | 111   | ASP  | 2.2  |
| 22  | QV    | 56    | C    | 2.2  |
| 5   | XE    | 46    | GLY  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | XK    | 15   | ALA  | 2.2  |
| 11  | XK    | 89   | ALA  | 2.2  |
| 17  | XQ    | 43   | LEU  | 2.2  |
| 19  | QS    | 82   | GLY  | 2.2  |
| 21  | QU    | 19   | GLY  | 2.2  |
| 31  | YH    | 161  | GLY  | 2.2  |
| 35  | YP    | 1    | MET  | 2.2  |
| 41  | YV    | 39   | LEU  | 2.2  |
| 45  | YZ    | 110  | GLY  | 2.2  |
| 50  | R4    | 64   | GLY  | 2.2  |
| 4   | QD    | 166  | LYS  | 2.2  |
| 8   | XH    | 116  | LYS  | 2.2  |
| 11  | XK    | 51   | LYS  | 2.2  |
| 12  | XL    | 114  | LYS  | 2.2  |
| 28  | YE    | 64   | LYS  | 2.2  |
| 33  | RN    | 89   | LYS  | 2.2  |
| 41  | YV    | 68   | LYS  | 2.2  |
| 7   | XG    | 156  | TRP  | 2.2  |
| 13  | QM    | 114  | ARG  | 2.2  |
| 27  | YD    | 273  | ARG  | 2.2  |
| 39  | RT    | 95   | ARG  | 2.2  |
| 43  | YX    | 68   | ARG  | 2.2  |
| 43  | RX    | 37   | THR  | 2.2  |
| 43  | YX    | 31   | HIS  | 2.2  |
| 17  | XQ    | 88   | TYR  | 2.2  |
| 39  | RT    | 32   | TYR  | 2.2  |
| 39  | RT    | 100  | TYR  | 2.2  |
| 4   | QD    | 8    | VAL  | 2.2  |
| 6   | QF    | 85   | VAL  | 2.2  |
| 12  | QL    | 55   | VAL  | 2.2  |
| 32  | RI    | 145  | VAL  | 2.2  |
| 42  | RW    | 13   | SER  | 2.2  |
| 50  | R4    | 26   | SER  | 2.2  |
| 1   | XA    | 1196 | U    | 2.2  |
| 5   | QE    | 141  | GLN  | 2.2  |
| 6   | QF    | 57   | GLN  | 2.2  |
| 11  | XK    | 104  | GLN  | 2.2  |
| 25  | RA    | 1420 | U    | 2.2  |
| 25  | YA    | 1420 | U    | 2.2  |
| 36  | RQ    | 12   | GLN  | 2.2  |
| 15  | QO    | 3    | ILE  | 2.2  |
| 29  | YF    | 206  | ILE  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | RS    | 18   | ILE  | 2.2  |
| 45  | YZ    | 146  | ILE  | 2.2  |
| 4   | XD    | 77   | ASN  | 2.2  |
| 1   | QA    | 1000 | A    | 2.2  |
| 1   | XA    | 1000 | A    | 2.2  |
| 25  | RA    | 2872 | G    | 2.2  |
| 25  | YA    | 1062 | G    | 2.2  |
| 29  | RF    | 161  | GLU  | 2.2  |
| 31  | YH    | 32   | GLU  | 2.2  |
| 36  | RQ    | 125  | LEU  | 2.2  |
| 41  | YV    | 15   | GLU  | 2.2  |
| 45  | RZ    | 178  | GLU  | 2.2  |
| 3   | QC    | 13   | GLY  | 2.2  |
| 5   | QE    | 29   | GLY  | 2.2  |
| 7   | XG    | 2    | ALA  | 2.2  |
| 11  | QK    | 58   | PRO  | 2.2  |
| 11  | XK    | 118  | GLY  | 2.2  |
| 45  | YZ    | 22   | GLY  | 2.2  |
| 50  | R4    | 29   | PRO  | 2.2  |
| 50  | Y4    | 12   | ALA  | 2.2  |
| 4   | XD    | 61   | LYS  | 2.2  |
| 32  | YI    | 110  | ASP  | 2.2  |
| 40  | RU    | 84   | LYS  | 2.2  |
| 45  | RZ    | 93   | ASP  | 2.2  |
| 51  | Y5    | 56   | LYS  | 2.2  |
| 2   | QB    | 122  | PHE  | 2.2  |
| 4   | XD    | 139  | ARG  | 2.2  |
| 18  | QR    | 43   | PHE  | 2.2  |
| 29  | RF    | 168  | ARG  | 2.2  |
| 50  | Y4    | 58   | ARG  | 2.2  |
| 1   | QA    | 1027 | C    | 2.2  |
| 25  | YA    | 34   | C    | 2.2  |
| 25  | YA    | 2178 | C    | 2.2  |
| 27  | YD    | 70   | TRP  | 2.2  |
| 8   | QH    | 24   | THR  | 2.2  |
| 10  | QJ    | 100  | THR  | 2.2  |
| 44  | RY    | 83   | THR  | 2.2  |
| 45  | RZ    | 151  | HIS  | 2.2  |
| 5   | QE    | 41   | VAL  | 2.2  |
| 9   | XI    | 108  | VAL  | 2.2  |
| 28  | YE    | 7    | VAL  | 2.2  |
| 29  | YF    | 154  | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | RH    | 49   | VAL  | 2.2  |
| 44  | YY    | 85   | VAL  | 2.2  |
| 7   | XG    | 86   | GLN  | 2.2  |
| 15  | QO    | 24   | SER  | 2.2  |
| 38  | RS    | 52   | SER  | 2.2  |
| 50  | R4    | 47   | GLN  | 2.2  |
| 50  | Y4    | 47   | GLN  | 2.2  |
| 20  | XT    | 10   | LEU  | 2.2  |
| 31  | RH    | 71   | LEU  | 2.2  |
| 32  | RI    | 116  | LEU  | 2.2  |
| 2   | QB    | 63   | MET  | 2.2  |
| 4   | QD    | 81   | GLU  | 2.2  |
| 7   | XG    | 7    | ALA  | 2.2  |
| 31  | YH    | 18   | GLU  | 2.2  |
| 28  | RE    | 64   | LYS  | 2.2  |
| 33  | RN    | 66   | LYS  | 2.2  |
| 35  | RP    | 124  | LYS  | 2.2  |
| 35  | YP    | 9    | ASN  | 2.2  |
| 35  | YP    | 89   | ALA  | 2.2  |
| 37  | RR    | 19   | ALA  | 2.2  |
| 38  | RS    | 86   | ALA  | 2.2  |
| 38  | YS    | 103  | GLU  | 2.2  |
| 39  | RT    | 21   | GLU  | 2.2  |
| 39  | RT    | 116  | ALA  | 2.2  |
| 39  | YT    | 38   | ASN  | 2.2  |
| 47  | Y1    | 93   | GLU  | 2.2  |
| 8   | QH    | 131  | GLY  | 2.2  |
| 15  | XO    | 89   | GLY  | 2.2  |
| 19  | QS    | 7    | LYS  | 2.2  |
| 19  | QS    | 8    | GLY  | 2.2  |
| 19  | QS    | 76   | PRO  | 2.2  |
| 21  | QU    | 12   | LYS  | 2.2  |
| 44  | RY    | 4    | LYS  | 2.2  |
| 44  | RY    | 63   | LYS  | 2.2  |
| 25  | RA    | 2189 | U    | 2.2  |
| 25  | YA    | 1097 | U    | 2.2  |
| 3   | XC    | 30   | ARG  | 2.2  |
| 11  | XK    | 120  | ARG  | 2.2  |
| 28  | RE    | 149  | ARG  | 2.2  |
| 36  | YQ    | 82   | ARG  | 2.2  |
| 25  | RA    | 1050 | A    | 2.2  |
| 25  | YA    | 74   | A    | 2.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 25  | YA    | 1086    | A    | 2.2  |
| 1   | QA    | 331     | G    | 2.2  |
| 1   | QA    | 1032(A) | G    | 2.2  |
| 1   | XA    | 1094    | G    | 2.2  |
| 25  | RA    | 2159    | G    | 2.2  |
| 25  | RA    | 2166    | G    | 2.2  |
| 25  | RA    | 2318    | G    | 2.2  |
| 25  | YA    | 1559    | G    | 2.2  |
| 4   | XD    | 125     | HIS  | 2.2  |
| 15  | QO    | 50      | HIS  | 2.2  |
| 4   | QD    | 121     | VAL  | 2.1  |
| 5   | XE    | 34      | VAL  | 2.1  |
| 8   | QH    | 120     | THR  | 2.1  |
| 17  | QQ    | 7       | THR  | 2.1  |
| 34  | RO    | 24      | VAL  | 2.1  |
| 45  | RZ    | 58      | VAL  | 2.1  |
| 49  | R3    | 59      | VAL  | 2.1  |
| 33  | YN    | 72      | TYR  | 2.1  |
| 45  | RZ    | 29      | TYR  | 2.1  |
| 1   | QA    | 962     | C    | 2.1  |
| 1   | XA    | 1195    | C    | 2.1  |
| 25  | YA    | 888     | C    | 2.1  |
| 55  | R9    | 10      | ILE  | 2.1  |
| 2   | XB    | 196     | LEU  | 2.1  |
| 3   | QC    | 178     | LEU  | 2.1  |
| 38  | RS    | 80      | LEU  | 2.1  |
| 44  | RY    | 14      | LEU  | 2.1  |
| 45  | RZ    | 18      | LEU  | 2.1  |
| 48  | Y2    | 53      | LEU  | 2.1  |
| 49  | R3    | 19      | GLN  | 2.1  |
| 17  | QQ    | 62      | SER  | 2.1  |
| 18  | QR    | 21      | LYS  | 2.1  |
| 19  | XS    | 7       | LYS  | 2.1  |
| 34  | YO    | 1       | MET  | 2.1  |
| 27  | RD    | 188     | GLU  | 2.1  |
| 35  | YP    | 120     | ALA  | 2.1  |
| 43  | RX    | 15      | GLU  | 2.1  |
| 44  | YY    | 62      | GLU  | 2.1  |
| 44  | YY    | 78      | ALA  | 2.1  |
| 45  | RZ    | 145     | GLU  | 2.1  |
| 45  | RZ    | 152     | ALA  | 2.1  |
| 45  | RZ    | 172     | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | RD    | 241  | PRO  | 2.1  |
| 30  | RG    | 83   | ARG  | 2.1  |
| 39  | YT    | 25   | GLY  | 2.1  |
| 46  | R0    | 55   | ARG  | 2.1  |
| 50  | Y4    | 3    | GLU  | 2.1  |
| 2   | QB    | 202  | PRO  | 2.1  |
| 4   | QD    | 37   | PRO  | 2.1  |
| 17  | QQ    | 54   | GLY  | 2.1  |
| 19  | QS    | 68   | GLY  | 2.1  |
| 31  | YH    | 5    | GLY  | 2.1  |
| 52  | R6    | 31   | PRO  | 2.1  |
| 53  | R7    | 38   | GLY  | 2.1  |
| 1   | QA    | 992  | U    | 2.1  |
| 5   | XE    | 5    | ASP  | 2.1  |
| 27  | RD    | 171  | ASP  | 2.1  |
| 42  | RW    | 67   | ASP  | 2.1  |
| 46  | R0    | 15   | ASP  | 2.1  |
| 7   | XG    | 153  | HIS  | 2.1  |
| 9   | XI    | 41   | VAL  | 2.1  |
| 12  | XL    | 18   | VAL  | 2.1  |
| 13  | QM    | 17   | VAL  | 2.1  |
| 19  | QS    | 60   | VAL  | 2.1  |
| 32  | RI    | 144  | VAL  | 2.1  |
| 44  | RY    | 42   | VAL  | 2.1  |
| 45  | RZ    | 27   | VAL  | 2.1  |
| 2   | XB    | 107  | THR  | 2.1  |
| 13  | QM    | 109  | THR  | 2.1  |
| 27  | YD    | 50   | THR  | 2.1  |
| 49  | Y3    | 40   | THR  | 2.1  |
| 3   | QC    | 182  | ILE  | 2.1  |
| 6   | XF    | 81   | ILE  | 2.1  |
| 7   | XG    | 42   | ILE  | 2.1  |
| 8   | QH    | 13   | ILE  | 2.1  |
| 13  | XM    | 84   | ILE  | 2.1  |
| 25  | RA    | 1085 | A    | 2.1  |
| 28  | RE    | 151  | TYR  | 2.1  |
| 36  | RQ    | 9    | TYR  | 2.1  |
| 45  | YZ    | 53   | ILE  | 2.1  |
| 55  | Y9    | 10   | ILE  | 2.1  |
| 55  | Y9    | 17   | ILE  | 2.1  |
| 9   | QI    | 56   | LEU  | 2.1  |
| 9   | XI    | 85   | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | XK    | 63   | LEU  | 2.1  |
| 12  | QL    | 115  | LYS  | 2.1  |
| 13  | QM    | 19   | LEU  | 2.1  |
| 16  | QP    | 35   | LYS  | 2.1  |
| 20  | QT    | 62   | LEU  | 2.1  |
| 28  | RE    | 8    | LYS  | 2.1  |
| 28  | RE    | 155  | LYS  | 2.1  |
| 31  | RH    | 153  | LYS  | 2.1  |
| 31  | YH    | 13   | LYS  | 2.1  |
| 33  | YN    | 2    | LYS  | 2.1  |
| 38  | RS    | 4    | LEU  | 2.1  |
| 41  | RV    | 85   | LYS  | 2.1  |
| 45  | RZ    | 150  | LEU  | 2.1  |
| 1   | QA    | 1178 | G    | 2.1  |
| 1   | XA    | 380  | G    | 2.1  |
| 1   | XA    | 481  | G    | 2.1  |
| 2   | XB    | 111  | ARG  | 2.1  |
| 3   | XC    | 180  | ALA  | 2.1  |
| 9   | QI    | 20   | ARG  | 2.1  |
| 10  | QJ    | 84   | GLN  | 2.1  |
| 11  | XK    | 93   | GLN  | 2.1  |
| 19  | QS    | 37   | ARG  | 2.1  |
| 25  | RA    | 352  | G    | 2.1  |
| 25  | RA    | 2792 | G    | 2.1  |
| 25  | YA    | 226  | G    | 2.1  |
| 25  | YA    | 2123 | G    | 2.1  |
| 37  | YR    | 1    | MET  | 2.1  |
| 31  | RH    | 152  | ARG  | 2.1  |
| 38  | RS    | 89   | ARG  | 2.1  |
| 38  | YS    | 30   | ARG  | 2.1  |
| 41  | YV    | 3    | ALA  | 2.1  |
| 47  | R1    | 61   | ARG  | 2.1  |
| 52  | Y6    | 44   | ARG  | 2.1  |
| 3   | XC    | 205  | GLY  | 2.1  |
| 1   | QA    | 1116 | C    | 2.1  |
| 1   | QA    | 1128 | C    | 2.1  |
| 1   | XA    | 63   | C    | 2.1  |
| 1   | XA    | 314  | C    | 2.1  |
| 1   | XA    | 1397 | C    | 2.1  |
| 19  | XS    | 2    | PRO  | 2.1  |
| 40  | YU    | 37   | GLU  | 2.1  |
| 43  | YX    | 38   | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | RZ    | 106  | GLY  | 2.1  |
| 50  | R4    | 54   | GLY  | 2.1  |
| 25  | YA    | 2161 | C    | 2.1  |
| 13  | QM    | 77   | ASN  | 2.1  |
| 14  | QN    | 16   | PHE  | 2.1  |
| 16  | QP    | 9    | PHE  | 2.1  |
| 39  | RT    | 76   | PHE  | 2.1  |
| 45  | RZ    | 30   | ASN  | 2.1  |
| 4   | XD    | 140  | VAL  | 2.1  |
| 12  | QL    | 112  | ASP  | 2.1  |
| 31  | RH    | 17   | VAL  | 2.1  |
| 34  | RO    | 63   | VAL  | 2.1  |
| 35  | RP    | 101  | VAL  | 2.1  |
| 27  | YD    | 58   | HIS  | 2.1  |
| 1   | XA    | 843  | U    | 2.1  |
| 4   | QD    | 207  | TYR  | 2.1  |
| 9   | XI    | 19   | LEU  | 2.1  |
| 13  | QM    | 63   | THR  | 2.1  |
| 19  | QS    | 30   | LEU  | 2.1  |
| 19  | XS    | 85   | LYS  | 2.1  |
| 25  | RA    | 1033 | U    | 2.1  |
| 25  | RA    | 1097 | U    | 2.1  |
| 26  | RB    | 103  | U    | 2.1  |
| 31  | RH    | 83   | TYR  | 2.1  |
| 32  | YI    | 9    | LEU  | 2.1  |
| 36  | RQ    | 130  | LYS  | 2.1  |
| 44  | YY    | 94   | LYS  | 2.1  |
| 45  | RZ    | 127  | LYS  | 2.1  |
| 45  | YZ    | 133  | ILE  | 2.1  |
| 50  | R4    | 24   | THR  | 2.1  |
| 55  | Y9    | 26   | ILE  | 2.1  |
| 4   | QD    | 14   | ARG  | 2.1  |
| 13  | QM    | 104  | ARG  | 2.1  |
| 18  | XR    | 54   | ARG  | 2.1  |
| 20  | XT    | 22   | ARG  | 2.1  |
| 39  | RT    | 54   | ARG  | 2.1  |
| 48  | R2    | 55   | ARG  | 2.1  |
| 54  | R8    | 30   | ARG  | 2.1  |
| 54  | R8    | 57   | ARG  | 2.1  |
| 10  | XJ    | 20   | ALA  | 2.1  |
| 30  | YG    | 6    | ALA  | 2.1  |
| 2   | QB    | 234  | PRO  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | XC    | 194  | GLY  | 2.1  |
| 4   | QD    | 150  | GLU  | 2.1  |
| 6   | XF    | 38   | GLU  | 2.1  |
| 13  | QM    | 69   | GLU  | 2.1  |
| 25  | YA    | 917  | A    | 2.1  |
| 28  | RE    | 50   | GLY  | 2.1  |
| 28  | YE    | 88   | GLY  | 2.1  |
| 28  | YE    | 193  | GLY  | 2.1  |
| 33  | RN    | 96   | GLU  | 2.1  |
| 35  | YP    | 69   | GLY  | 2.1  |
| 39  | RT    | 4    | GLY  | 2.1  |
| 50  | Y4    | 4    | GLY  | 2.1  |
| 36  | RQ    | 65   | PHE  | 2.1  |
| 45  | RZ    | 88   | PHE  | 2.1  |
| 40  | RU    | 75   | ASN  | 2.1  |
| 48  | Y2    | 47   | ASN  | 2.1  |
| 52  | R6    | 29   | ASN  | 2.1  |
| 1   | QA    | 377  | G    | 2.1  |
| 1   | QA    | 1184 | G    | 2.1  |
| 1   | XA    | 6    | G    | 2.1  |
| 1   | XA    | 610  | G    | 2.1  |
| 25  | YA    | 2127 | G    | 2.1  |
| 25  | YA    | 2211 | G    | 2.1  |
| 25  | YA    | 2751 | G    | 2.1  |
| 31  | RH    | 76   | VAL  | 2.1  |
| 45  | RZ    | 116  | VAL  | 2.1  |
| 1   | QA    | 150  | C    | 2.1  |
| 25  | YA    | 2791 | C    | 2.1  |
| 4   | QD    | 102  | ASP  | 2.1  |
| 5   | QE    | 123  | LEU  | 2.1  |
| 6   | QF    | 14   | LEU  | 2.1  |
| 7   | QG    | 33   | ASP  | 2.1  |
| 20  | QT    | 87   | LYS  | 2.1  |
| 29  | YF    | 77   | ASP  | 2.1  |
| 33  | RN    | 127  | ASP  | 2.1  |
| 45  | RZ    | 144  | LEU  | 2.1  |
| 45  | YZ    | 140  | ASP  | 2.1  |
| 47  | Y1    | 96   | LYS  | 2.1  |
| 9   | XI    | 63   | ILE  | 2.1  |
| 10  | QJ    | 75   | ILE  | 2.1  |
| 14  | QN    | 40   | CYS  | 2.1  |
| 7   | XG    | 79   | ARG  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | QK    | 75   | TYR  | 2.1  |
| 19  | XS    | 48   | THR  | 2.1  |
| 30  | RG    | 115  | ARG  | 2.1  |
| 39  | RT    | 93   | ARG  | 2.1  |
| 50  | Y4    | 55   | ARG  | 2.1  |
| 27  | YD    | 9    | TYR  | 2.1  |
| 36  | RQ    | 115  | MET  | 2.1  |
| 12  | XL    | 128  | ALA  | 2.1  |
| 32  | RI    | 65   | ALA  | 2.1  |
| 35  | RP    | 150  | ALA  | 2.1  |
| 36  | RQ    | 20   | ALA  | 2.1  |
| 25  | RA    | 2150 | U    | 2.1  |
| 16  | QP    | 63   | GLY  | 2.1  |
| 28  | YE    | 125  | GLY  | 2.1  |
| 29  | RF    | 55   | GLY  | 2.1  |
| 41  | YV    | 67   | GLY  | 2.1  |
| 2   | XB    | 105  | PHE  | 2.1  |
| 5   | QE    | 122  | GLU  | 2.1  |
| 28  | RE    | 22   | PRO  | 2.1  |
| 39  | RT    | 81   | PRO  | 2.1  |
| 40  | RU    | 108  | GLU  | 2.1  |
| 30  | RG    | 78   | SER  | 2.1  |
| 31  | RH    | 134  | SER  | 2.1  |
| 47  | R1    | 49   | VAL  | 2.1  |
| 2   | XB    | 94   | ASN  | 2.1  |
| 25  | RA    | 1460 | A    | 2.1  |
| 25  | YA    | 1070 | A    | 2.1  |
| 25  | YA    | 1510 | A    | 2.1  |
| 2   | QB    | 200  | ILE  | 2.1  |
| 3   | QC    | 127  | ARG  | 2.1  |
| 13  | QM    | 78   | ILE  | 2.1  |
| 13  | XM    | 56   | LEU  | 2.1  |
| 4   | QD    | 123  | HIS  | 2.1  |
| 14  | XN    | 19   | ARG  | 2.1  |
| 20  | QT    | 86   | ARG  | 2.1  |
| 35  | YP    | 90   | ARG  | 2.1  |
| 42  | RW    | 111  | HIS  | 2.1  |
| 44  | RY    | 97   | ARG  | 2.1  |
| 44  | YY    | 86   | ARG  | 2.1  |
| 27  | RD    | 230  | ASP  | 2.1  |
| 31  | RH    | 137  | ASP  | 2.1  |
| 36  | YQ    | 135  | ASP  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 5   | QE    | 120    | THR  | 2.1  |
| 11  | XK    | 50     | TYR  | 2.1  |
| 47  | Y1    | 35     | THR  | 2.1  |
| 50  | Y4    | 24     | THR  | 2.1  |
| 1   | QA    | 570    | G    | 2.1  |
| 1   | QA    | 1271   | G    | 2.1  |
| 2   | XB    | 77     | ALA  | 2.1  |
| 13  | QM    | 118    | ALA  | 2.1  |
| 25  | RA    | 2178   | C    | 2.1  |
| 25  | YA    | 654(B) | C    | 2.1  |
| 22  | QV    | 10     | G    | 2.1  |
| 23  | QY    | 42     | G    | 2.1  |
| 25  | RA    | 274    | G    | 2.1  |
| 25  | RA    | 1091   | G    | 2.1  |
| 25  | YA    | 1728   | G    | 2.1  |
| 27  | RD    | 153    | ALA  | 2.1  |
| 51  | R5    | 18     | ALA  | 2.1  |
| 7   | XG    | 106    | GLN  | 2.1  |
| 10  | XJ    | 93     | GLY  | 2.1  |
| 16  | QP    | 10     | GLY  | 2.1  |
| 20  | XT    | 102    | GLY  | 2.1  |
| 36  | RQ    | 13     | GLN  | 2.1  |
| 2   | XB    | 26     | PRO  | 2.1  |
| 4   | XD    | 15     | GLU  | 2.1  |
| 4   | XD    | 110    | PHE  | 2.1  |
| 6   | QF    | 41     | GLU  | 2.1  |
| 6   | QF    | 60     | PHE  | 2.1  |
| 14  | XN    | 16     | PHE  | 2.1  |
| 17  | QQ    | 86     | GLU  | 2.1  |
| 27  | RD    | 15     | PHE  | 2.1  |
| 32  | RI    | 117    | GLU  | 2.1  |
| 33  | YN    | 10     | GLU  | 2.1  |
| 45  | YZ    | 169    | GLU  | 2.1  |
| 4   | XD    | 203    | VAL  | 2.0  |
| 9   | XI    | 127    | LYS  | 2.0  |
| 13  | XM    | 115    | LYS  | 2.0  |
| 22  | QV    | 47     | U    | 2.0  |
| 25  | YA    | 1372   | U    | 2.0  |
| 25  | YA    | 2506   | U    | 2.0  |
| 27  | RD    | 26     | LYS  | 2.0  |
| 27  | YD    | 34     | VAL  | 2.0  |
| 31  | RH    | 19     | VAL  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | RH    | 140  | LYS  | 2.0  |
| 31  | YH    | 52   | VAL  | 2.0  |
| 31  | YH    | 140  | LYS  | 2.0  |
| 32  | YI    | 145  | VAL  | 2.0  |
| 45  | YZ    | 141  | VAL  | 2.0  |
| 50  | Y4    | 10   | VAL  | 2.0  |
| 17  | XQ    | 62   | SER  | 2.0  |
| 39  | RT    | 80   | SER  | 2.0  |
| 2   | XB    | 130  | ARG  | 2.0  |
| 2   | XB    | 138  | LEU  | 2.0  |
| 3   | XC    | 164  | ARG  | 2.0  |
| 8   | QH    | 10   | LEU  | 2.0  |
| 8   | XH    | 112  | LEU  | 2.0  |
| 9   | XI    | 40   | LEU  | 2.0  |
| 11  | QK    | 126  | ARG  | 2.0  |
| 13  | QM    | 57   | ARG  | 2.0  |
| 14  | QN    | 7    | ILE  | 2.0  |
| 17  | QQ    | 6    | LEU  | 2.0  |
| 19  | XS    | 37   | ARG  | 2.0  |
| 20  | XT    | 100  | ILE  | 2.0  |
| 27  | YD    | 203  | ASN  | 2.0  |
| 32  | YI    | 77   | LEU  | 2.0  |
| 38  | YS    | 110  | LEU  | 2.0  |
| 49  | R3    | 8    | LEU  | 2.0  |
| 49  | Y3    | 30   | ARG  | 2.0  |
| 50  | Y4    | 22   | ILE  | 2.0  |
| 32  | RI    | 1    | MET  | 2.0  |
| 37  | RR    | 50   | HIS  | 2.0  |
| 2   | QB    | 171  | ALA  | 2.0  |
| 10  | QJ    | 89   | ASP  | 2.0  |
| 16  | XP    | 38   | TYR  | 2.0  |
| 25  | RA    | 1098 | A    | 2.0  |
| 25  | RA    | 1210 | A    | 2.0  |
| 25  | YA    | 655  | A    | 2.0  |
| 32  | YI    | 100  | ALA  | 2.0  |
| 35  | RP    | 89   | ALA  | 2.0  |
| 35  | RP    | 127  | ALA  | 2.0  |
| 50  | R4    | 44   | THR  | 2.0  |
| 3   | QC    | 159  | GLY  | 2.0  |
| 10  | QJ    | 21   | GLN  | 2.0  |
| 17  | QQ    | 26   | GLN  | 2.0  |
| 27  | YD    | 135  | PHE  | 2.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 31  | YH    | 91     | GLY  | 2.0  |
| 35  | YP    | 104    | GLY  | 2.0  |
| 39  | RT    | 90     | GLN  | 2.0  |
| 54  | R8    | 38     | GLY  | 2.0  |
| 12  | QL    | 71     | PRO  | 2.0  |
| 1   | QA    | 1096   | C    | 2.0  |
| 3   | QC    | 4      | LYS  | 2.0  |
| 31  | RH    | 77     | LYS  | 2.0  |
| 45  | RZ    | 2      | GLU  | 2.0  |
| 51  | Y5    | 48     | GLU  | 2.0  |
| 55  | Y9    | 13     | LYS  | 2.0  |
| 28  | RE    | 72     | VAL  | 2.0  |
| 31  | RH    | 113    | VAL  | 2.0  |
| 1   | QA    | 108    | G    | 2.0  |
| 1   | QA    | 1224   | G    | 2.0  |
| 1   | XA    | 129(A) | G    | 2.0  |
| 1   | XA    | 1053   | G    | 2.0  |
| 1   | XA    | 1202   | G    | 2.0  |
| 3   | QC    | 43     | LEU  | 2.0  |
| 5   | XE    | 40     | ARG  | 2.0  |
| 11  | QK    | 12     | ARG  | 2.0  |
| 19  | QS    | 15     | LEU  | 2.0  |
| 25  | YA    | 2792   | G    | 2.0  |
| 25  | YA    | 2795   | G    | 2.0  |
| 34  | YO    | 104    | ARG  | 2.0  |
| 36  | YQ    | 6      | ARG  | 2.0  |
| 36  | YQ    | 60     | ARG  | 2.0  |
| 37  | YR    | 33     | ARG  | 2.0  |
| 38  | YS    | 10     | ARG  | 2.0  |
| 40  | RU    | 11     | ARG  | 2.0  |
| 40  | YU    | 92     | ARG  | 2.0  |
| 52  | R6    | 6      | ARG  | 2.0  |
| 54  | R8    | 50     | LEU  | 2.0  |
| 4   | QD    | 67     | ILE  | 2.0  |
| 4   | XD    | 158    | ILE  | 2.0  |
| 4   | XD    | 175    | SER  | 2.0  |
| 10  | QJ    | 38     | ILE  | 2.0  |
| 10  | XJ    | 75     | ILE  | 2.0  |
| 10  | XJ    | 96     | ILE  | 2.0  |
| 15  | XO    | 24     | SER  | 2.0  |
| 31  | RH    | 38     | SER  | 2.0  |
| 31  | YH    | 9      | ILE  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | RY    | 96   | ILE  | 2.0  |
| 1   | QA    | 5    | U    | 2.0  |
| 1   | QA    | 1196 | U    | 2.0  |
| 1   | XA    | 992  | U    | 2.0  |
| 19  | XS    | 65   | ASN  | 2.0  |
| 22  | XV    | 20   | U    | 2.0  |
| 25  | YA    | 1175 | U    | 2.0  |
| 6   | XF    | 62   | TRP  | 2.0  |
| 10  | XJ    | 56   | HIS  | 2.0  |
| 20  | QT    | 56   | MET  | 2.0  |
| 28  | RE    | 1    | MET  | 2.0  |
| 33  | RN    | 130  | HIS  | 2.0  |
| 3   | XC    | 15   | THR  | 2.0  |
| 5   | QE    | 21   | ALA  | 2.0  |
| 7   | QG    | 2    | ALA  | 2.0  |
| 8   | XH    | 28   | ALA  | 2.0  |
| 9   | QI    | 5    | TYR  | 2.0  |
| 9   | QI    | 114  | TYR  | 2.0  |
| 13  | XM    | 116  | THR  | 2.0  |
| 29  | RF    | 177  | ALA  | 2.0  |
| 41  | YV    | 49   | THR  | 2.0  |
| 44  | RY    | 65   | ALA  | 2.0  |
| 43  | RX    | 5    | TYR  | 2.0  |
| 45  | RZ    | 99   | TYR  | 2.0  |
| 4   | XD    | 134  | ASP  | 2.0  |
| 28  | YE    | 127  | ASP  | 2.0  |
| 3   | XC    | 10   | PHE  | 2.0  |
| 5   | QE    | 124  | GLY  | 2.0  |
| 11  | QK    | 118  | GLY  | 2.0  |
| 17  | QQ    | 71   | PHE  | 2.0  |
| 33  | YN    | 64   | GLY  | 2.0  |
| 36  | RQ    | 15   | GLY  | 2.0  |
| 4   | XD    | 182  | LYS  | 2.0  |
| 5   | QE    | 47   | LYS  | 2.0  |
| 7   | QG    | 58   | PRO  | 2.0  |
| 7   | QG    | 88   | PRO  | 2.0  |
| 12  | QL    | 114  | LYS  | 2.0  |
| 31  | RH    | 139  | GLN  | 2.0  |
| 33  | YN    | 69   | GLN  | 2.0  |
| 34  | RO    | 66   | LYS  | 2.0  |
| 35  | RP    | 64   | LYS  | 2.0  |
| 38  | RS    | 59   | LYS  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | RS    | 93   | LYS  | 2.0  |
| 39  | YT    | 136  | GLN  | 2.0  |
| 1   | XA    | 162  | A    | 2.0  |
| 3   | XC    | 46   | GLU  | 2.0  |
| 6   | QF    | 87   | ARG  | 2.0  |
| 9   | QI    | 28   | VAL  | 2.0  |
| 11  | QK    | 92   | GLU  | 2.0  |
| 13  | QM    | 60   | VAL  | 2.0  |
| 29  | YF    | 179  | GLU  | 2.0  |
| 47  | Y1    | 75   | GLU  | 2.0  |
| 49  | R3    | 57   | GLU  | 2.0  |
| 14  | QN    | 35   | ARG  | 2.0  |
| 28  | RE    | 61   | ARG  | 2.0  |
| 3   | QC    | 101  | LEU  | 2.0  |
| 4   | XD    | 64   | LEU  | 2.0  |
| 16  | XP    | 49   | LEU  | 2.0  |
| 29  | RF    | 32   | LEU  | 2.0  |
| 52  | Y6    | 10   | LEU  | 2.0  |
| 5   | XE    | 129  | ILE  | 2.0  |
| 7   | QG    | 42   | ILE  | 2.0  |
| 12  | XL    | 85   | ILE  | 2.0  |
| 31  | RH    | 151  | ILE  | 2.0  |
| 1   | QA    | 328  | C    | 2.0  |
| 1   | XA    | 1322 | C    | 2.0  |
| 22  | QV    | 16   | C    | 2.0  |
| 22  | XV    | 68   | C    | 2.0  |
| 25  | YA    | 1072 | C    | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 56  | PPU  | Z8    | 76  | 37/38 | 0.84 | 0.27 | 70,70,70,70                | 0     |
| 56  | PPU  | Z6    | 76  | 37/38 | 0.86 | 0.25 | 73,73,73,73                | 0     |
| 23  | 1MG  | QY    | 37  | 24/25 | 0.90 | 0.12 | 86,86,86,86                | 0     |
| 23  | 1MG  | XY    | 37  | 24/25 | 0.93 | 0.11 | 62,62,62,62                | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSR  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3085 | 1/1   | 0.12 | 0.52 | 65,65,65,65                 | 0     |
| 57  | MG   | RA    | 3193 | 1/1   | 0.18 | 0.21 | 114,114,114,114             | 0     |
| 57  | MG   | QA    | 1625 | 1/1   | 0.18 | 0.24 | 94,94,94,94                 | 0     |
| 57  | MG   | RA    | 3130 | 1/1   | 0.22 | 0.26 | 94,94,94,94                 | 0     |
| 57  | MG   | RA    | 3194 | 1/1   | 0.27 | 0.28 | 96,96,96,96                 | 0     |
| 57  | MG   | RA    | 3120 | 1/1   | 0.30 | 0.41 | 89,89,89,89                 | 0     |
| 57  | MG   | QA    | 1657 | 1/1   | 0.32 | 0.27 | 108,108,108,108             | 0     |
| 57  | MG   | RA    | 3139 | 1/1   | 0.33 | 0.32 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3218 | 1/1   | 0.38 | 0.26 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3115 | 1/1   | 0.42 | 0.26 | 47,47,47,47                 | 0     |
| 57  | MG   | QA    | 1608 | 1/1   | 0.42 | 0.24 | 68,68,68,68                 | 0     |
| 57  | MG   | YA    | 3132 | 1/1   | 0.42 | 0.29 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3122 | 1/1   | 0.43 | 0.45 | 95,95,95,95                 | 0     |
| 57  | MG   | YA    | 3129 | 1/1   | 0.47 | 0.21 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3062 | 1/1   | 0.47 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3167 | 1/1   | 0.48 | 0.29 | 42,42,42,42                 | 0     |
| 57  | MG   | QF    | 201  | 1/1   | 0.56 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | RA    | 3163 | 1/1   | 0.57 | 0.27 | 79,79,79,79                 | 0     |
| 57  | MG   | YA    | 3220 | 1/1   | 0.59 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | QA    | 1617 | 1/1   | 0.60 | 0.35 | 50,50,50,50                 | 0     |
| 57  | MG   | QX    | 101  | 1/1   | 0.61 | 0.15 | 67,67,67,67                 | 0     |
| 57  | MG   | YA    | 3141 | 1/1   | 0.61 | 0.24 | 79,79,79,79                 | 0     |
| 57  | MG   | XA    | 1638 | 1/1   | 0.61 | 0.25 | 91,91,91,91                 | 0     |
| 57  | MG   | XA    | 1670 | 1/1   | 0.61 | 0.11 | 79,79,79,79                 | 0     |
| 57  | MG   | XA    | 1608 | 1/1   | 0.62 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3117 | 1/1   | 0.62 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | YP    | 201  | 1/1   | 0.62 | 0.16 | 153,153,153,153             | 0     |
| 57  | MG   | YA    | 3082 | 1/1   | 0.63 | 0.76 | 80,80,80,80                 | 0     |
| 57  | MG   | XA    | 1664 | 1/1   | 0.65 | 0.27 | 84,84,84,84                 | 0     |
| 57  | MG   | XA    | 1673 | 1/1   | 0.65 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | RA    | 3228 | 1/1   | 0.67 | 0.18 | 91,91,91,91                 | 0     |
| 57  | MG   | RA    | 3223 | 1/1   | 0.67 | 0.18 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3207 | 1/1   | 0.68 | 0.40 | 105,105,105,105             | 0     |
| 57  | MG   | RA    | 3199 | 1/1   | 0.69 | 0.24 | 72,72,72,72                 | 0     |
| 57  | MG   | YA    | 3072 | 1/1   | 0.69 | 0.20 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3156 | 1/1   | 0.69 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3177 | 1/1   | 0.69 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3226 | 1/1   | 0.71 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3195 | 1/1   | 0.71 | 0.24 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3204 | 1/1   | 0.71 | 0.10 | 63,63,63,63                 | 0     |
| 57  | MG   | QA    | 1649 | 1/1   | 0.71 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3180 | 1/1   | 0.72 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | QA    | 1609 | 1/1   | 0.72 | 0.03 | 14,14,14,14                 | 0     |
| 57  | MG   | QH    | 201  | 1/1   | 0.73 | 0.09 | 74,74,74,74                 | 0     |
| 57  | MG   | RA    | 3135 | 1/1   | 0.73 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | RA    | 3221 | 1/1   | 0.73 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | XA    | 1619 | 1/1   | 0.74 | 0.24 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3220 | 1/1   | 0.74 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3203 | 1/1   | 0.74 | 0.25 | 61,61,61,61                 | 0     |
| 57  | MG   | RA    | 3233 | 1/1   | 0.74 | 0.26 | 42,42,42,42                 | 0     |
| 57  | MG   | R0    | 101  | 1/1   | 0.74 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3242 | 1/1   | 0.74 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3068 | 1/1   | 0.74 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3157 | 1/1   | 0.75 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3155 | 1/1   | 0.75 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | QA    | 1663 | 1/1   | 0.75 | 0.12 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3091 | 1/1   | 0.75 | 0.31 | 65,65,65,65                 | 0     |
| 57  | MG   | QA    | 1637 | 1/1   | 0.76 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | QA    | 1627 | 1/1   | 0.76 | 0.32 | 92,92,92,92                 | 0     |
| 57  | MG   | YP    | 202  | 1/1   | 0.76 | 0.20 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3162 | 1/1   | 0.77 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3101 | 1/1   | 0.77 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | XA    | 1634 | 1/1   | 0.77 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | XA    | 1614 | 1/1   | 0.77 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | YA    | 3223 | 1/1   | 0.78 | 0.24 | 42,42,42,42                 | 0     |
| 57  | MG   | XA    | 1620 | 1/1   | 0.78 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | XA    | 1629 | 1/1   | 0.79 | 0.22 | 44,44,44,44                 | 0     |
| 57  | MG   | YB    | 204  | 1/1   | 0.79 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3103 | 1/1   | 0.79 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3191 | 1/1   | 0.79 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | XA    | 1660 | 1/1   | 0.80 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | YB    | 202  | 1/1   | 0.80 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | RB    | 202  | 1/1   | 0.80 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3084 | 1/1   | 0.80 | 0.16 | 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   | QA    | 1618 | 1/1   | 0.80 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3150 | 1/1   | 0.81 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3166 | 1/1   | 0.81 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | XA    | 1624 | 1/1   | 0.81 | 0.26 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3248 | 1/1   | 0.81 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | QA    | 1656 | 1/1   | 0.81 | 0.13 | 100,100,100,100             | 0     |
| 57  | MG   | RA    | 3118 | 1/1   | 0.81 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3011 | 1/1   | 0.81 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | XA    | 1639 | 1/1   | 0.81 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3169 | 1/1   | 0.82 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | QA    | 1645 | 1/1   | 0.82 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3229 | 1/1   | 0.82 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | RA    | 3078 | 1/1   | 0.82 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | XA    | 1631 | 1/1   | 0.82 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3221 | 1/1   | 0.83 | 0.41 | 42,42,42,42                 | 0     |
| 57  | MG   | QA    | 1614 | 1/1   | 0.83 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3130 | 1/1   | 0.83 | 0.25 | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3184 | 1/1   | 0.83 | 0.23 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3044 | 1/1   | 0.83 | 0.24 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3222 | 1/1   | 0.83 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3206 | 1/1   | 0.83 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | RA    | 3138 | 1/1   | 0.83 | 0.19 | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3175 | 1/1   | 0.84 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | XA    | 1665 | 1/1   | 0.84 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | YA    | 3224 | 1/1   | 0.84 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3230 | 1/1   | 0.84 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3107 | 1/1   | 0.84 | 0.16 | 41,41,41,41                 | 0     |
| 58  | PAR  | QA    | 1666 | 42/42 | 0.84 | 0.26 | 84,84,84,84                 | 0     |
| 58  | PAR  | XA    | 1675 | 42/42 | 0.84 | 0.21 | 74,74,74,74                 | 0     |
| 57  | MG   | QA    | 1660 | 1/1   | 0.85 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3133 | 1/1   | 0.85 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | XA    | 1648 | 1/1   | 0.85 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | XA    | 1650 | 1/1   | 0.85 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3127 | 1/1   | 0.85 | 0.10 | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3165 | 1/1   | 0.85 | 0.29 | 43,43,43,43                 | 0     |
| 57  | MG   | QA    | 1628 | 1/1   | 0.85 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | RA    | 3167 | 1/1   | 0.85 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | QA    | 1640 | 1/1   | 0.85 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3143 | 1/1   | 0.85 | 0.23 | 66,66,66,66                 | 0     |
| 57  | MG   | YA    | 3149 | 1/1   | 0.85 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3250 | 1/1   | 0.85 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3075 | 1/1   | 0.85 | 0.10 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3016 | 1/1   | 0.85 | 0.13 | 20,20,20,20                 | 0     |
| 57  | MG   | RA    | 3121 | 1/1   | 0.85 | 0.23 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3076 | 1/1   | 0.85 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3174 | 1/1   | 0.85 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | RD    | 301  | 1/1   | 0.85 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1636 | 1/1   | 0.86 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3131 | 1/1   | 0.86 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3188 | 1/1   | 0.86 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3011 | 1/1   | 0.86 | 0.22 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3142 | 1/1   | 0.86 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | RA    | 3059 | 1/1   | 0.86 | 0.18 | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3182 | 1/1   | 0.86 | 0.33 | 55,55,55,55                 | 0     |
| 57  | MG   | YA    | 3265 | 1/1   | 0.86 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | XA    | 1656 | 1/1   | 0.86 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | YA    | 3193 | 1/1   | 0.86 | 0.20 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3168 | 1/1   | 0.86 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | XA    | 1661 | 1/1   | 0.86 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3212 | 1/1   | 0.86 | 0.31 | 67,67,67,67                 | 0     |
| 57  | MG   | RA    | 3122 | 1/1   | 0.86 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | QA    | 1654 | 1/1   | 0.87 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | YA    | 3201 | 1/1   | 0.87 | 0.31 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3127 | 1/1   | 0.87 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3008 | 1/1   | 0.87 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3171 | 1/1   | 0.87 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | RA    | 3211 | 1/1   | 0.87 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3212 | 1/1   | 0.87 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3151 | 1/1   | 0.87 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3154 | 1/1   | 0.87 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3234 | 1/1   | 0.87 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | QA    | 1655 | 1/1   | 0.87 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3157 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3091 | 1/1   | 0.87 | 0.13 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3097 | 1/1   | 0.87 | 0.23 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3106 | 1/1   | 0.87 | 0.13 | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3160 | 1/1   | 0.87 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3185 | 1/1   | 0.87 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3023 | 1/1   | 0.87 | 0.26 | 8,8,8,8                     | 0     |
| 57  | MG   | QA    | 1646 | 1/1   | 0.87 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | QA    | 1629 | 1/1   | 0.87 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3155 | 1/1   | 0.88 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | RA    | 3094 | 1/1   | 0.88 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | QA    | 1650 | 1/1   | 0.88 | 0.15 | 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    | 3253 | 1/1   | 0.88 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3047 | 1/1   | 0.88 | 0.19 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3064 | 1/1   | 0.88 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | XA    | 1636 | 1/1   | 0.88 | 0.27 | 23,23,23,23                 | 0     |
| 57  | MG   | QA    | 1606 | 1/1   | 0.88 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3229 | 1/1   | 0.88 | 0.13 | 20,20,20,20                 | 0     |
| 57  | MG   | XA    | 1621 | 1/1   | 0.88 | 0.28 | 32,32,32,32                 | 0     |
| 57  | MG   | RA    | 3019 | 1/1   | 0.88 | 0.17 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3069 | 1/1   | 0.89 | 0.24 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3207 | 1/1   | 0.89 | 0.27 | 52,52,52,52                 | 0     |
| 57  | MG   | XA    | 1652 | 1/1   | 0.89 | 0.11 | 64,64,64,64                 | 0     |
| 57  | MG   | YA    | 3218 | 1/1   | 0.89 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | QA    | 1631 | 1/1   | 0.89 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | XA    | 1658 | 1/1   | 0.89 | 0.23 | 61,61,61,61                 | 0     |
| 57  | MG   | QA    | 1644 | 1/1   | 0.89 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | RE    | 301  | 1/1   | 0.89 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3092 | 1/1   | 0.89 | 0.15 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3082 | 1/1   | 0.89 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | QV    | 101  | 1/1   | 0.89 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3163 | 1/1   | 0.89 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3166 | 1/1   | 0.89 | 0.23 | 55,55,55,55                 | 0     |
| 57  | MG   | XA    | 1637 | 1/1   | 0.89 | 0.19 | 39,39,39,39                 | 0     |
| 57  | MG   | RA    | 3173 | 1/1   | 0.89 | 0.16 | 90,90,90,90                 | 0     |
| 57  | MG   | RA    | 3195 | 1/1   | 0.89 | 0.23 | 85,85,85,85                 | 0     |
| 57  | MG   | RA    | 3114 | 1/1   | 0.89 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3046 | 1/1   | 0.89 | 0.17 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3236 | 1/1   | 0.89 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | XA    | 1651 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | YA    | 3136 | 1/1   | 0.89 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3139 | 1/1   | 0.89 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3189 | 1/1   | 0.90 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3217 | 1/1   | 0.90 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | YA    | 3030 | 1/1   | 0.90 | 0.31 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3170 | 1/1   | 0.90 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | XA    | 1649 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3048 | 1/1   | 0.90 | 0.27 | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3126 | 1/1   | 0.90 | 0.45 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3214 | 1/1   | 0.90 | 0.09 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3148 | 1/1   | 0.90 | 0.27 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3148 | 1/1   | 0.90 | 0.27 | 39,39,39,39                 | 0     |
| 57  | MG   | QA    | 1662 | 1/1   | 0.90 | 0.06 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3180 | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | XA    | 1657 | 1/1   | 0.90 | 0.31 | 48,48,48,48                 | 0     |
| 57  | MG   | YA    | 3152 | 1/1   | 0.90 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3224 | 1/1   | 0.90 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3137 | 1/1   | 0.90 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3205 | 1/1   | 0.90 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | QA    | 1639 | 1/1   | 0.90 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | RA    | 3208 | 1/1   | 0.90 | 0.13 | 69,69,69,69                 | 0     |
| 57  | MG   | RA    | 3210 | 1/1   | 0.90 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3115 | 1/1   | 0.90 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | QM    | 201  | 1/1   | 0.90 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | XA    | 1674 | 1/1   | 0.90 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3176 | 1/1   | 0.90 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3124 | 1/1   | 0.90 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | YA    | 3125 | 1/1   | 0.90 | 0.25 | 65,65,65,65                 | 0     |
| 57  | MG   | YA    | 3186 | 1/1   | 0.90 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | QA    | 1620 | 1/1   | 0.91 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3158 | 1/1   | 0.91 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3131 | 1/1   | 0.91 | 0.19 | 15,15,15,15                 | 0     |
| 57  | MG   | RB    | 201  | 1/1   | 0.91 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3199 | 1/1   | 0.91 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3181 | 1/1   | 0.91 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | QA    | 1612 | 1/1   | 0.91 | 0.27 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3111 | 1/1   | 0.91 | 0.14 | 20,20,20,20                 | 0     |
| 57  | MG   | RR    | 202  | 1/1   | 0.91 | 0.11 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3146 | 1/1   | 0.91 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | QA    | 1619 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3079 | 1/1   | 0.91 | 0.20 | 18,18,18,18                 | 0     |
| 57  | MG   | XA    | 1654 | 1/1   | 0.91 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | QA    | 1632 | 1/1   | 0.91 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3077 | 1/1   | 0.91 | 0.17 | 24,24,24,24                 | 0     |
| 57  | MG   | XA    | 1618 | 1/1   | 0.91 | 0.24 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3032 | 1/1   | 0.91 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3103 | 1/1   | 0.91 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3160 | 1/1   | 0.91 | 0.09 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3243 | 1/1   | 0.91 | 0.28 | 32,32,32,32                 | 0     |
| 57  | MG   | RA    | 3041 | 1/1   | 0.91 | 0.17 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3249 | 1/1   | 0.91 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3196 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | YA    | 3108 | 1/1   | 0.91 | 0.19 | 20,20,20,20                 | 0     |
| 57  | MG   | QA    | 1664 | 1/1   | 0.91 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3055 | 1/1   | 0.91 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | XA    | 1630 | 1/1   | 0.91 | 0.16 | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3057 | 1/1   | 0.91 | 0.21 | 34,34,34,34                 | 0     |
| 57  | MG   | RA    | 3175 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3230 | 1/1   | 0.91 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3184 | 1/1   | 0.91 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3021 | 1/1   | 0.92 | 0.21 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3022 | 1/1   | 0.92 | 0.25 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3168 | 1/1   | 0.92 | 0.29 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3169 | 1/1   | 0.92 | 0.06 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3172 | 1/1   | 0.92 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | QA    | 1661 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | RA    | 3132 | 1/1   | 0.92 | 0.19 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3235 | 1/1   | 0.92 | 0.24 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3177 | 1/1   | 0.92 | 0.29 | 71,71,71,71                 | 0     |
| 57  | MG   | RA    | 3197 | 1/1   | 0.92 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3066 | 1/1   | 0.92 | 0.18 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3200 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3110 | 1/1   | 0.92 | 0.25 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3114 | 1/1   | 0.92 | 0.18 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3026 | 1/1   | 0.92 | 0.10 | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3112 | 1/1   | 0.92 | 0.17 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3198 | 1/1   | 0.92 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | QA    | 1635 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | RA    | 3206 | 1/1   | 0.92 | 0.31 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3202 | 1/1   | 0.92 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | XA    | 1607 | 1/1   | 0.92 | 0.18 | 25,25,25,25                 | 0     |
| 57  | MG   | XA    | 1667 | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | RA    | 3009 | 1/1   | 0.92 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | XA    | 1671 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3042 | 1/1   | 0.92 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3209 | 1/1   | 0.92 | 0.07 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3119 | 1/1   | 0.92 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3222 | 1/1   | 0.92 | 0.26 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3176 | 1/1   | 0.92 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3149 | 1/1   | 0.92 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3142 | 1/1   | 0.92 | 0.19 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3045 | 1/1   | 0.92 | 0.29 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3216 | 1/1   | 0.92 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3238 | 1/1   | 0.92 | 0.26 | 154,154,154,154             | 0     |
| 57  | MG   | YA    | 3239 | 1/1   | 0.92 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3179 | 1/1   | 0.92 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3151 | 1/1   | 0.92 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | YA    | 3244 | 1/1   | 0.92 | 0.19 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3050 | 1/1   | 0.92 | 0.17 | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3061 | 1/1   | 0.92 | 0.17 | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3080 | 1/1   | 0.92 | 0.22 | 15,15,15,15                 | 0     |
| 57  | MG   | QA    | 1643 | 1/1   | 0.92 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | QA    | 1601 | 1/1   | 0.92 | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | YA    | 3268 | 1/1   | 0.92 | 0.28 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3075 | 1/1   | 0.92 | 0.09 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3088 | 1/1   | 0.92 | 0.22 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3161 | 1/1   | 0.92 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3159 | 1/1   | 0.92 | 0.29 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3191 | 1/1   | 0.92 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3164 | 1/1   | 0.92 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | QA    | 1665 | 1/1   | 0.93 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | XA    | 1659 | 1/1   | 0.93 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | YA    | 3203 | 1/1   | 0.93 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | QA    | 1615 | 1/1   | 0.93 | 0.07 | 66,66,66,66                 | 0     |
| 57  | MG   | XA    | 1626 | 1/1   | 0.93 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3214 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3237 | 1/1   | 0.93 | 0.20 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3215 | 1/1   | 0.93 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3217 | 1/1   | 0.93 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3106 | 1/1   | 0.93 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3125 | 1/1   | 0.93 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | XA    | 1635 | 1/1   | 0.93 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | RA    | 3161 | 1/1   | 0.93 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3027 | 1/1   | 0.93 | 0.22 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3003 | 1/1   | 0.93 | 0.11 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3225 | 1/1   | 0.93 | 0.16 | 21,21,21,21                 | 0     |
| 57  | MG   | RF    | 301  | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | YA    | 3014 | 1/1   | 0.93 | 0.20 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3231 | 1/1   | 0.93 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3048 | 1/1   | 0.93 | 0.23 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3021 | 1/1   | 0.93 | 0.20 | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3121 | 1/1   | 0.93 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | XA    | 1640 | 1/1   | 0.93 | 0.09 | 187,187,187,187             | 0     |
| 57  | MG   | YA    | 3042 | 1/1   | 0.93 | 0.22 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3050 | 1/1   | 0.93 | 0.23 | 13,13,13,13                 | 0     |
| 57  | MG   | R5    | 101  | 1/1   | 0.93 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3150 | 1/1   | 0.93 | 0.23 | 32,32,32,32                 | 0     |
| 57  | MG   | RA    | 3186 | 1/1   | 0.93 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3251 | 1/1   | 0.93 | 0.34 | 60,60,60,60                 | 0     |
| 57  | MG   | YA    | 3252 | 1/1   | 0.93 | 0.33 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3052 | 1/1   | 0.93 | 0.12 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3152 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3133 | 1/1   | 0.93 | 0.16 | 12,12,12,12                 | 0     |
| 57  | MG   | YB    | 201  | 1/1   | 0.93 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | YA    | 3134 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | YB    | 203  | 1/1   | 0.93 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | XA    | 1655 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | YE    | 301  | 1/1   | 0.93 | 0.14 | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3065 | 1/1   | 0.93 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3092 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3002 | 1/1   | 0.93 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | YA    | 3074 | 1/1   | 0.93 | 0.20 | 22,22,22,22                 | 0     |
| 59  | ZN   | QN    | 101  | 1/1   | 0.93 | 0.07 | 87,87,87,87                 | 0     |
| 57  | MG   | RA    | 3099 | 1/1   | 0.94 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | RE    | 302  | 1/1   | 0.94 | 0.08 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3095 | 1/1   | 0.94 | 0.19 | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3100 | 1/1   | 0.94 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | YA    | 3178 | 1/1   | 0.94 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3179 | 1/1   | 0.94 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3102 | 1/1   | 0.94 | 0.28 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3181 | 1/1   | 0.94 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3030 | 1/1   | 0.94 | 0.17 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3104 | 1/1   | 0.94 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3012 | 1/1   | 0.94 | 0.09 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3035 | 1/1   | 0.94 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | XA    | 1606 | 1/1   | 0.94 | 0.24 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3109 | 1/1   | 0.94 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3112 | 1/1   | 0.94 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3037 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3200 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | XA    | 1669 | 1/1   | 0.94 | 0.11 | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3013 | 1/1   | 0.94 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3119 | 1/1   | 0.94 | 0.15 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3144 | 1/1   | 0.94 | 0.19 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3213 | 1/1   | 0.94 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3210 | 1/1   | 0.94 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3211 | 1/1   | 0.94 | 0.13 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3145 | 1/1   | 0.94 | 0.17 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3001 | 1/1   | 0.94 | 0.19 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3113 | 1/1   | 0.94 | 0.15 | 22,22,22,22                 | 0     |
| 57  | MG   | YA    | 3009 | 1/1   | 0.94 | 0.27 | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1611 | 1/1   | 0.94 | 0.14 | 20,20,20,20                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3043 | 1/1   | 0.94 | 0.11 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3079 | 1/1   | 0.94 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3018 | 1/1   | 0.94 | 0.22 | 6,6,6,6                     | 0     |
| 57  | MG   | QA    | 1648 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3135 | 1/1   | 0.94 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3023 | 1/1   | 0.94 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3137 | 1/1   | 0.94 | 0.11 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3024 | 1/1   | 0.94 | 0.28 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3027 | 1/1   | 0.94 | 0.19 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3007 | 1/1   | 0.94 | 0.17 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3035 | 1/1   | 0.94 | 0.23 | 12,12,12,12                 | 0     |
| 57  | MG   | XA    | 1632 | 1/1   | 0.94 | 0.22 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3147 | 1/1   | 0.94 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | XA    | 1633 | 1/1   | 0.94 | 0.23 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3083 | 1/1   | 0.94 | 0.17 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3245 | 1/1   | 0.94 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | QA    | 1603 | 1/1   | 0.94 | 0.22 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3192 | 1/1   | 0.94 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3227 | 1/1   | 0.94 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | YA    | 3153 | 1/1   | 0.94 | 0.33 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3060 | 1/1   | 0.94 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3123 | 1/1   | 0.94 | 0.18 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3256 | 1/1   | 0.94 | 0.14 | 11,11,11,11                 | 0     |
| 57  | MG   | QA    | 1616 | 1/1   | 0.94 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3267 | 1/1   | 0.94 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3158 | 1/1   | 0.94 | 0.17 | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1658 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | XA    | 1641 | 1/1   | 0.94 | 0.21 | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3028 | 1/1   | 0.94 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3128 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | RA    | 3164 | 1/1   | 0.94 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3129 | 1/1   | 0.94 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3201 | 1/1   | 0.94 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3202 | 1/1   | 0.94 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3058 | 1/1   | 0.94 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3088 | 1/1   | 0.94 | 0.25 | 17,17,17,17                 | 0     |
| 59  | ZN   | R9    | 101  | 1/1   | 0.94 | 0.08 | 112,112,112,112             | 0     |
| 57  | MG   | QA    | 1652 | 1/1   | 0.95 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3031 | 1/1   | 0.95 | 0.27 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3032 | 1/1   | 0.95 | 0.19 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3034 | 1/1   | 0.95 | 0.22 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3096 | 1/1   | 0.95 | 0.15 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3040 | 1/1   | 0.95 | 0.09 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3204 | 1/1   | 0.95 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | QA    | 1653 | 1/1   | 0.95 | 0.06 | 82,82,82,82                 | 0     |
| 57  | MG   | RA    | 3240 | 1/1   | 0.95 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | XA    | 1645 | 1/1   | 0.95 | 0.19 | 30,30,30,30                 | 0     |
| 57  | MG   | QA    | 1613 | 1/1   | 0.95 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3056 | 1/1   | 0.95 | 0.21 | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3136 | 1/1   | 0.95 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3056 | 1/1   | 0.95 | 0.12 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3058 | 1/1   | 0.95 | 0.22 | 11,11,11,11                 | 0     |
| 57  | MG   | QA    | 1604 | 1/1   | 0.95 | 0.18 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3219 | 1/1   | 0.95 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3172 | 1/1   | 0.95 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | XA    | 1653 | 1/1   | 0.95 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | QA    | 1642 | 1/1   | 0.95 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3108 | 1/1   | 0.95 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | QA    | 1621 | 1/1   | 0.95 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3073 | 1/1   | 0.95 | 0.12 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3227 | 1/1   | 0.95 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | RA    | 3001 | 1/1   | 0.95 | 0.06 | 2,2,2,2                     | 0     |
| 57  | MG   | XA    | 1603 | 1/1   | 0.95 | 0.22 | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3178 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3156 | 1/1   | 0.95 | 0.06 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3236 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3237 | 1/1   | 0.95 | 0.17 | 9,9,9,9                     | 0     |
| 57  | MG   | QA    | 1622 | 1/1   | 0.95 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3146 | 1/1   | 0.95 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3084 | 1/1   | 0.95 | 0.18 | 6,6,6,6                     | 0     |
| 57  | MG   | XA    | 1663 | 1/1   | 0.95 | 0.30 | 35,35,35,35                 | 0     |
| 57  | MG   | XA    | 1611 | 1/1   | 0.95 | 0.19 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3215 | 1/1   | 0.95 | 0.13 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3247 | 1/1   | 0.95 | 0.20 | 26,26,26,26                 | 0     |
| 57  | MG   | XA    | 1616 | 1/1   | 0.95 | 0.23 | 14,14,14,14                 | 0     |
| 57  | MG   | XA    | 1668 | 1/1   | 0.95 | 0.22 | 30,30,30,30                 | 0     |
| 57  | MG   | QA    | 1659 | 1/1   | 0.95 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3071 | 1/1   | 0.95 | 0.18 | 18,18,18,18                 | 0     |
| 57  | MG   | QA    | 1623 | 1/1   | 0.95 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | QA    | 1634 | 1/1   | 0.95 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3254 | 1/1   | 0.95 | 0.24 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3038 | 1/1   | 0.95 | 0.10 | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3260 | 1/1   | 0.95 | 0.19 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3262 | 1/1   | 0.95 | 0.31 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | QA    | 1624 | 1/1   | 0.95 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | XA    | 1627 | 1/1   | 0.95 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | QA    | 1610 | 1/1   | 0.95 | 0.20 | 22,22,22,22                 | 0     |
| 57  | MG   | QA    | 1626 | 1/1   | 0.95 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3012 | 1/1   | 0.95 | 0.17 | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3225 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3014 | 1/1   | 0.95 | 0.17 | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3046 | 1/1   | 0.95 | 0.14 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3120 | 1/1   | 0.95 | 0.16 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3087 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | Y0    | 101  | 1/1   | 0.95 | 0.17 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3189 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3047 | 1/1   | 0.95 | 0.24 | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3015 | 1/1   | 0.95 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3049 | 1/1   | 0.95 | 0.09 | 14,14,14,14                 | 0     |
| 59  | ZN   | Y9    | 101  | 1/1   | 0.95 | 0.07 | 87,87,87,87                 | 0     |
| 57  | MG   | QA    | 1647 | 1/1   | 0.96 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | RA    | 3004 | 1/1   | 0.96 | 0.10 | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3116 | 1/1   | 0.96 | 0.11 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3197 | 1/1   | 0.96 | 0.17 | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3085 | 1/1   | 0.96 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3238 | 1/1   | 0.96 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3140 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3141 | 1/1   | 0.96 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | YA    | 3028 | 1/1   | 0.96 | 0.10 | 3,3,3,3                     | 0     |
| 57  | MG   | QA    | 1602 | 1/1   | 0.96 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3143 | 1/1   | 0.96 | 0.04 | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3126 | 1/1   | 0.96 | 0.16 | 17,17,17,17                 | 0     |
| 57  | MG   | XA    | 1642 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3209 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3128 | 1/1   | 0.96 | 0.28 | 34,34,34,34                 | 0     |
| 57  | MG   | YA    | 3033 | 1/1   | 0.96 | 0.17 | 10,10,10,10                 | 0     |
| 57  | MG   | XA    | 1643 | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3213 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | XA    | 1644 | 1/1   | 0.96 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3039 | 1/1   | 0.96 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3065 | 1/1   | 0.96 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | XA    | 1647 | 1/1   | 0.96 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3174 | 1/1   | 0.96 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | RA    | 3016 | 1/1   | 0.96 | 0.15 | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3034 | 1/1   | 0.96 | 0.26 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3093 | 1/1   | 0.96 | 0.18 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3069 | 1/1   | 0.96 | 0.06 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3053 | 1/1   | 0.96 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3055 | 1/1   | 0.96 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3226 | 1/1   | 0.96 | 0.05 | 20,20,20,20                 | 0     |
| 57  | MG   | XA    | 1602 | 1/1   | 0.96 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3095 | 1/1   | 0.96 | 0.17 | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3124 | 1/1   | 0.96 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | QA    | 1607 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3232 | 1/1   | 0.96 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3233 | 1/1   | 0.96 | 0.20 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3063 | 1/1   | 0.96 | 0.11 | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3235 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3182 | 1/1   | 0.96 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | XA    | 1610 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3068 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | RA    | 3183 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3241 | 1/1   | 0.96 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | XA    | 1612 | 1/1   | 0.96 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3154 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | XA    | 1662 | 1/1   | 0.96 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | XA    | 1615 | 1/1   | 0.96 | 0.31 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3097 | 1/1   | 0.96 | 0.15 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3098 | 1/1   | 0.96 | 0.16 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3187 | 1/1   | 0.96 | 0.05 | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3072 | 1/1   | 0.96 | 0.14 | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3073 | 1/1   | 0.96 | 0.10 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3165 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3086 | 1/1   | 0.96 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | XA    | 1622 | 1/1   | 0.96 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3089 | 1/1   | 0.96 | 0.13 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3257 | 1/1   | 0.96 | 0.17 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3259 | 1/1   | 0.96 | 0.23 | 14,14,14,14                 | 0     |
| 57  | MG   | XA    | 1623 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3036 | 1/1   | 0.96 | 0.13 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3173 | 1/1   | 0.96 | 0.34 | 32,32,32,32                 | 0     |
| 57  | MG   | QA    | 1605 | 1/1   | 0.96 | 0.25 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3053 | 1/1   | 0.96 | 0.16 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3098 | 1/1   | 0.96 | 0.14 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3101 | 1/1   | 0.96 | 0.25 | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3162 | 1/1   | 0.96 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3006 | 1/1   | 0.96 | 0.19 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3008 | 1/1   | 0.96 | 0.16 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3010 | 1/1   | 0.96 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | QA    | 1630 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3183 | 1/1   | 0.96 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | QA    | 1641 | 1/1   | 0.96 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | YA    | 3013 | 1/1   | 0.96 | 0.15 | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3187 | 1/1   | 0.96 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3198 | 1/1   | 0.96 | 0.15 | 22,22,22,22                 | 0     |
| 59  | ZN   | XN    | 101  | 1/1   | 0.96 | 0.10 | 103,103,103,103             | 0     |
| 57  | MG   | YA    | 3190 | 1/1   | 0.96 | 0.08 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3216 | 1/1   | 0.97 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3041 | 1/1   | 0.97 | 0.15 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3031 | 1/1   | 0.97 | 0.14 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3044 | 1/1   | 0.97 | 0.21 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3159 | 1/1   | 0.97 | 0.08 | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3051 | 1/1   | 0.97 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3105 | 1/1   | 0.97 | 0.09 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3153 | 1/1   | 0.97 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | RA    | 3086 | 1/1   | 0.97 | 0.14 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3110 | 1/1   | 0.97 | 0.07 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3109 | 1/1   | 0.97 | 0.14 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3049 | 1/1   | 0.97 | 0.14 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3228 | 1/1   | 0.97 | 0.09 | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3025 | 1/1   | 0.97 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3134 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | YA    | 3054 | 1/1   | 0.97 | 0.17 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3170 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | YA    | 3171 | 1/1   | 0.97 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3003 | 1/1   | 0.97 | 0.22 | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1646 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3118 | 1/1   | 0.97 | 0.29 | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3089 | 1/1   | 0.97 | 0.11 | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3059 | 1/1   | 0.97 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3234 | 1/1   | 0.97 | 0.22 | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3240 | 1/1   | 0.97 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3070 | 1/1   | 0.97 | 0.11 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3123 | 1/1   | 0.97 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | YA    | 3062 | 1/1   | 0.97 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3054 | 1/1   | 0.97 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | QA    | 1633 | 1/1   | 0.97 | 0.20 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3246 | 1/1   | 0.97 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3045 | 1/1   | 0.97 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3015 | 1/1   | 0.97 | 0.18 | 3,3,3,3                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3185 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | QA    | 1638 | 1/1   | 0.97 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | YA    | 3070 | 1/1   | 0.97 | 0.14 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3188 | 1/1   | 0.97 | 0.04 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3017 | 1/1   | 0.97 | 0.14 | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3029 | 1/1   | 0.97 | 0.14 | 6,6,6,6                     | 0     |
| 57  | MG   | QA    | 1651 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3190 | 1/1   | 0.97 | 0.04 | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3194 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | XA    | 1628 | 1/1   | 0.97 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3261 | 1/1   | 0.97 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3078 | 1/1   | 0.97 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3060 | 1/1   | 0.97 | 0.15 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3138 | 1/1   | 0.97 | 0.12 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3061 | 1/1   | 0.97 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | RA    | 3081 | 1/1   | 0.97 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3147 | 1/1   | 0.97 | 0.05 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3219 | 1/1   | 0.97 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3040 | 1/1   | 0.97 | 0.16 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3205 | 1/1   | 0.97 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | RA    | 3102 | 1/1   | 0.97 | 0.18 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3090 | 1/1   | 0.97 | 0.15 | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3063 | 1/1   | 0.97 | 0.29 | 12,12,12,12                 | 0     |
| 57  | MG   | Y5    | 101  | 1/1   | 0.97 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3036 | 1/1   | 0.97 | 0.18 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3093 | 1/1   | 0.97 | 0.09 | 18,18,18,18                 | 0     |
| 59  | ZN   | QD    | 301  | 1/1   | 0.97 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | YA    | 3038 | 1/1   | 0.97 | 0.14 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3096 | 1/1   | 0.97 | 0.18 | 7,7,7,7                     | 0     |
| 59  | ZN   | XD    | 301  | 1/1   | 0.97 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | XA    | 1666 | 1/1   | 0.97 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | XA    | 1605 | 1/1   | 0.97 | 0.15 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3067 | 1/1   | 0.98 | 0.10 | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3005 | 1/1   | 0.98 | 0.22 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3006 | 1/1   | 0.98 | 0.15 | 7,7,7,7                     | 0     |
| 57  | MG   | XA    | 1601 | 1/1   | 0.98 | 0.16 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3087 | 1/1   | 0.98 | 0.13 | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3017 | 1/1   | 0.98 | 0.10 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3051 | 1/1   | 0.98 | 0.15 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3019 | 1/1   | 0.98 | 0.11 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3090 | 1/1   | 0.98 | 0.04 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3022 | 1/1   | 0.98 | 0.15 | 11,11,11,11                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | XA    | 1625 | 1/1   | 0.98 | 0.06 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3057 | 1/1   | 0.98 | 0.07 | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3039 | 1/1   | 0.98 | 0.09 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3026 | 1/1   | 0.98 | 0.21 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3064 | 1/1   | 0.98 | 0.21 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3258 | 1/1   | 0.98 | 0.19 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3100 | 1/1   | 0.98 | 0.13 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3116 | 1/1   | 0.98 | 0.10 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3117 | 1/1   | 0.98 | 0.05 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3140 | 1/1   | 0.98 | 0.10 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3263 | 1/1   | 0.98 | 0.10 | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1672 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3266 | 1/1   | 0.98 | 0.16 | 11,11,11,11                 | 0     |
| 57  | MG   | XA    | 1609 | 1/1   | 0.98 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3241 | 1/1   | 0.98 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | YA    | 3144 | 1/1   | 0.98 | 0.05 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3145 | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3066 | 1/1   | 0.98 | 0.06 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3067 | 1/1   | 0.98 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3018 | 1/1   | 0.98 | 0.11 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3002 | 1/1   | 0.98 | 0.20 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3104 | 1/1   | 0.98 | 0.04 | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3111 | 1/1   | 0.98 | 0.04 | 5,5,5,5                     | 0     |
| 57  | MG   | XA    | 1613 | 1/1   | 0.98 | 0.04 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3105 | 1/1   | 0.98 | 0.09 | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3024 | 1/1   | 0.98 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3010 | 1/1   | 0.98 | 0.06 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3107 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3077 | 1/1   | 0.98 | 0.24 | 11,11,11,11                 | 0     |
| 57  | MG   | XA    | 1617 | 1/1   | 0.98 | 0.12 | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3076 | 1/1   | 0.98 | 0.11 | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3081 | 1/1   | 0.98 | 0.22 | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3232 | 1/1   | 0.99 | 0.25 | 23,23,23,23                 | 0     |
| 57  | MG   | YA    | 3264 | 1/1   | 0.99 | 0.15 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3007 | 1/1   | 0.99 | 0.09 | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3025 | 1/1   | 0.99 | 0.05 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3037 | 1/1   | 0.99 | 0.06 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3033 | 1/1   | 0.99 | 0.24 | 11,11,11,11                 | 0     |
| 57  | MG   | RR    | 201  | 1/1   | 0.99 | 0.10 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3113 | 1/1   | 0.99 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3052 | 1/1   | 0.99 | 0.09 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3080 | 1/1   | 0.99 | 0.06 | 11,11,11,11                 | 0     |

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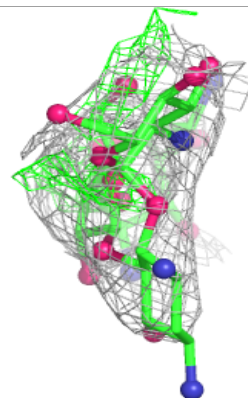
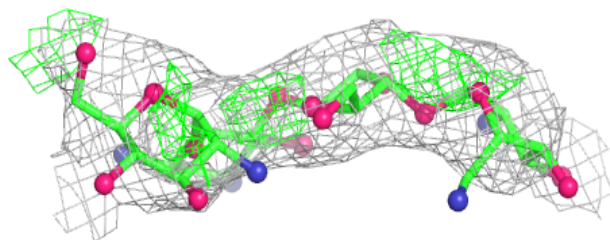
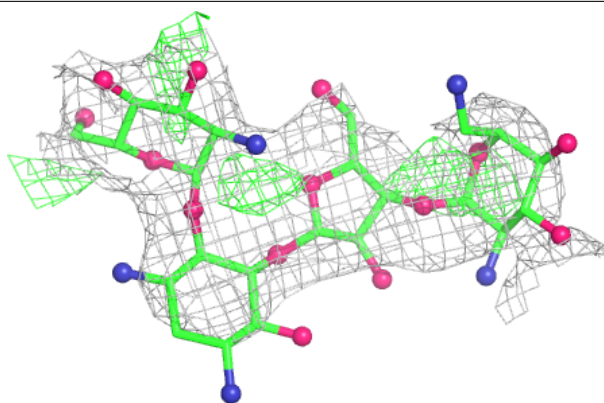
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3208 | 1/1   | 0.99 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | XA    | 1604 | 1/1   | 0.99 | 0.23 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3099 | 1/1   | 0.99 | 0.09 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3074 | 1/1   | 0.99 | 0.06 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3083 | 1/1   | 0.99 | 0.06 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3255 | 1/1   | 0.99 | 0.24 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3192 | 1/1   | 0.99 | 0.04 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3020 | 1/1   | 0.99 | 0.23 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3043 | 1/1   | 0.99 | 0.11 | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3239 | 1/1   | 0.99 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | YA    | 3196 | 1/1   | 0.99 | 0.03 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3071 | 1/1   | 0.99 | 0.04 | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3231 | 1/1   | 0.99 | 0.17 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3020 | 1/1   | 1.00 | 0.09 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3004 | 1/1   | 1.00 | 0.05 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3029 | 1/1   | 1.00 | 0.06 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3094 | 1/1   | 1.00 | 0.02 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3005 | 1/1   | 1.00 | 0.03 | 7,7,7,7                     | 0     |

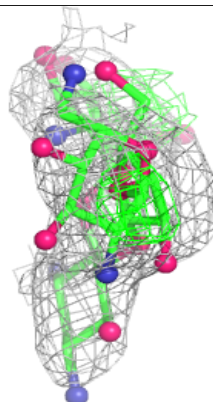
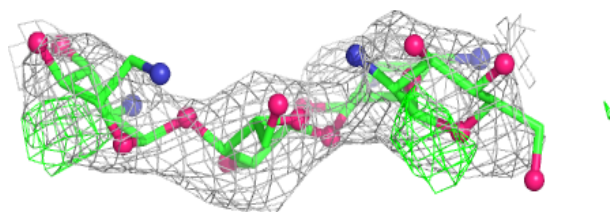
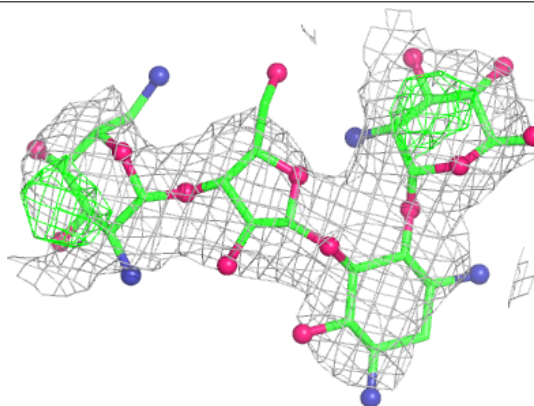
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PAR QA 1666:**

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

**Electron density around PAR XA 1675:**

$2mF_o-DF_c$  (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.